

Paul Schuleritz please

Access DB# 103705

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SABHA QAZI Examined: 74141 Date: 9/11/03
Art Unit: 1616 Phone Number 305-3910 Serial Number: 09/497,891
Mail Box and Bldg/Room Location: 2019 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

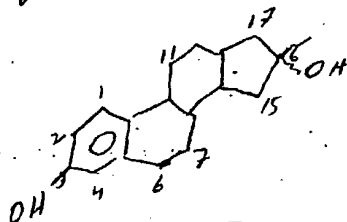
Title of Invention: 3,16-dihydroxyestra 1,3,5,(10) triene

Inventors (please provide full names): HERMAN KUENZER et al.

Earliest Priority Filing Date: 2/4/2000 DE 19906159

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for compds of formula in Cl 53
3,16 dihydroxyestra 1,3,5(10)-triene derivative



Please note, ^①no hydroxyl on 17-position
R¹⁷ may be H, X, alkyl, ester or ester derivative

^② R⁷, X, H, alkyl, alkoxy.
You may leave other positions open?

Thank you.
Compds of Cl 64 can be searched separately

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: _____	NA Sequence (#) _____	STN <u>793.22</u>
Searcher Phone #: _____	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <u>3</u>	Questel/Orbit _____
Date Searcher Picked Up: <u>9/12</u>	Bibliographic _____	Dr. Link _____
Date Completed: <u>9/25/03</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: <u>30</u>	Fulltext _____	Sequence Systems _____
Clerical Prep Time: _____	Patent Family _____	WWW/Internet _____
Online Time: <u>27</u>	Other _____	Other (specify) _____

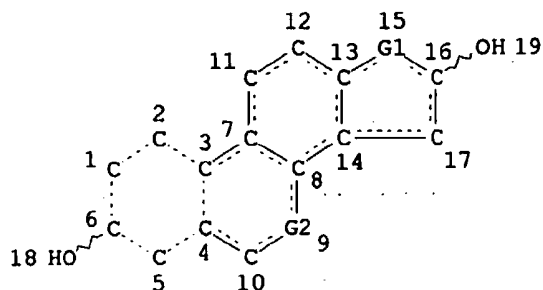
Claim 69

Qazi 09/497,891

September 25, 2003

=> d que
L1

STR



CH~X
@20 21

CH~Ak
@22 23

CH~X
@24 25

CH~Ak
@26 27

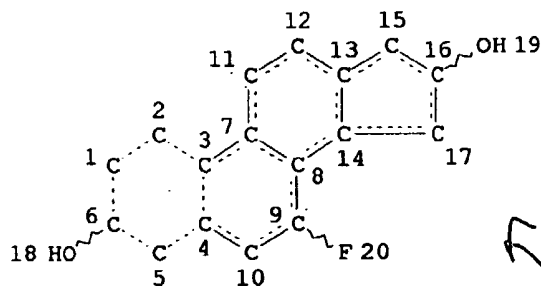
CH~O~Ak
@28 29 30

18α-homo-estra-1,3,5(10)-triene-3,16α-diol
not found

VAR G1=CH2/20/22
VAR G2=CH2/24/26/28
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE
L3 203 SEA FILE=REGISTRY SSS FUL L1
L13 STR

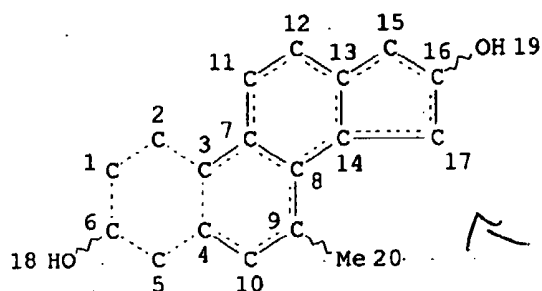


7α fluoro...

NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L14 2 SEA FILE=REGISTRY SUB=L3 SSS FUL L13
L15 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L16 2 SEA FILE=REGISTRY SUB=L3 SSS FUL L15
 L23 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L14 OR L16

=> d 1010 abs 111511

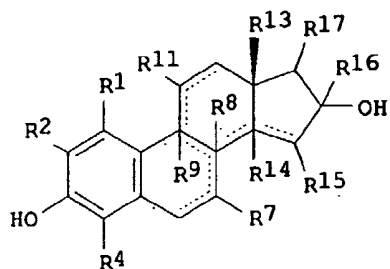
L23 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 2000:552017 HCAPLUS
 DOCUMENT NUMBER: 133:150782
 TITLE: synthesis of 16-Hydroxyestratrienes as selectively effective estrogens
 INVENTOR(S): Kuenzer, Hermann; Knauth, Rudolf; Lessl, Monika; Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa; Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk
 PATENT ASSIGNEE(S): Schering A.-G., Germany
 SOURCE: Ger. Offen., 34 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

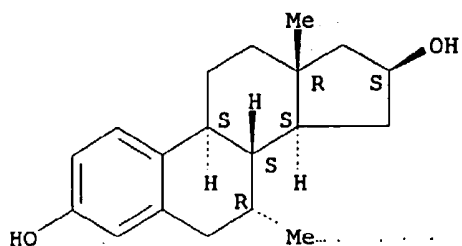
AU 2000029095	A5	20000829	AU 2000-29095	20000209
EP 1144431	A2	20011017	EP 2000-907539	20000209
EP 1144431	A3	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008076	A	20020205	BR 2000-8076	20000209
JP 2002536455	T2	20021029	JP 2000-598520	20000209
EE 200100412	A	20021216	EE 2001-412	20000209
NO 2001003860	A	20011008	NO 2001-3860	20010808
BG 105804	A	20020329	BG 2001-105804	20010809
PRIORITY APPLN. INFO.:			DE 1999-19906159 A	19990209
OTHER SOURCE(S):			WO 2000-EP1073 W	20000209
GI			MARPAT 133:150782	



I

- AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2, CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16.alpha.-estradiol shows a 50% uterine stimulation at 30 .upsilon.g in in vivo testing.
- IT 287721-57-7P 287721-58-8P 287721-71-5P
287721-85-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective estrogens)
- RN 287721-57-7 HCAPLUS
- CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

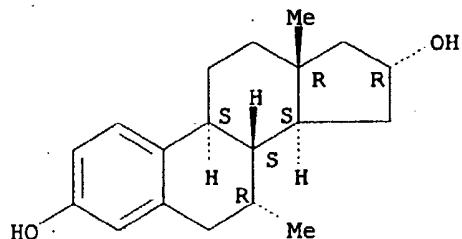
Absolute stereochemistry. Rotation (+).



RN 287721-58-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

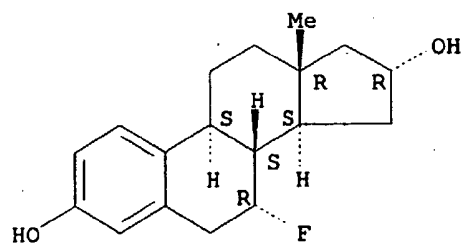
Absolute stereochemistry. Rotation (+).



RN 287721-71-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

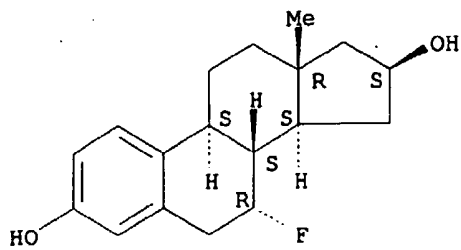
Absolute stereochemistry.



RN 287721-85-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



Claim 53

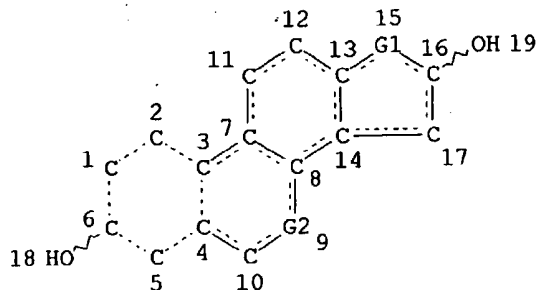
Qazi 09/497,891

September 25, 2003

=> d que 15

L1

STR



CH~X
@20 21

CH~Ak
@22 23

CH~X
@24 25

CH~Ak
@26 27

CH~O~Ak
@28 29 30

VAR G1=CH2/20/22

VAR G2=CH2/24/26/28

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

L3 203 SEA FILE=REGISTRY SSS FUL L1

L5 90 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d ibib-ab hitstr l5 1-90

L5 ANSWER 1 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:717656 HCAPLUS

DOCUMENT NUMBER: 138:50028

TITLE: Development and validation of an average mammalian estrogen receptor-based QSAR model

AUTHOR(S): Mekenyan, O.; Kamenska, V.; Serafimova, R.; Poellinger, L.; Brouwer, A.; Walker, J.

CORPORATE SOURCE: Laboratory of Mathematical Chemistry, University "As. Zlatarov", Bourgas, 8010, Bulg.

SOURCE: SAR and QSAR in Environmental Research (2002), 13(6), 579-595

CODEN: SQERED; ISSN: 1062-936X

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Development and evaluation of quant. structure activity relationships (QSARs) for predicting estrogen receptor binding from chem. structure requires reliable algorithms for three-dimensional (3D) QSAR anal. and establishment of structurally diverse training sets of chems. whose modes of action and measures of potency are well defined. One approach to

selecting an appropriate training set is to minimize the biol. variability in the model development, by using structurally restricted data sets. A second approach is to extend the structural diversity of chems. at the cost of increased variability of biol. assays. In this study, the second approach was used by organizing a training set of 151 chems. with measured human alpha Estrogen Receptor (ER.alpha.), mouse uterine, rat uterine, and MCF7 cell Relative Binding Affinities (RBAs). The structurally augmented training set was submitted to a 3D pattern recognition anal. to derive a model for av. mammalian ER binding affinity by employing the Common REactivity Pattern (COREPA) approach. Elucidation of this pattern required examn. of the conformational flexibility of the compds. to reveal areas in the multidimensional descriptor space, which are most populated by the conformers of the biol. active mols. and least populated by the inactive ones. The approach is not dependent upon a predetd. and specified toxicophore or an alignment of conformers to a lead compd. Reactivity patterns assocd. with mammalian ER binding affinity were obtained in terms of global nucleophilicity (EHOMO), interat. distances between nucleophilic sites, and local nucleophilicity (charges or delocalizabilities) of those sites. Based on derived patterns, descriptor profiles were established for identifying and ranking compds. with RBA of >150, 150-10, 10-1 and 1-0.1% relative to 17.beta.-estradiol. Specificity of reactivity profiles was found to increase gradually with increasing affinities assocd. with RBAs ranges under study. Using the results of this anal., an exploratory expert system was developed for use in ranking relative mammalian ER binding affinity potential for large chem. data sets. The validity of the RBA predictions were confirmed by independent development and comparison with measured RBA values.

IT 1090-04-6, 16.alpha.-Estradiol

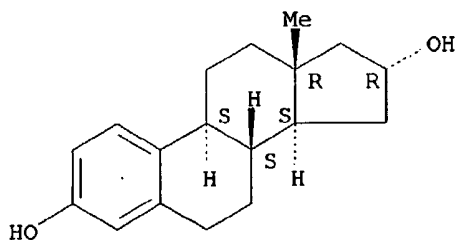
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(development and validation of an av. mammalian estrogen receptor-based QSAR model)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:122822 HCAPLUS

DOCUMENT NUMBER: 136:161698

TITLE: Combination preparation with an ER.beta. selective estrogen and a SERM or antiestrogen

INVENTOR(S): Fritzemeier, Karl-Heinrich; Kollenkirchen, Uwe;

PATENT ASSIGNEE(S): Hegele-Hartung, Christa
 SOURCE: Schering Aktiengesellschaft, Germany
 PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002011765	A1	20020214	WO 2001-EP9008	20010803
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10039199	A1	20020221	DE 2000-10039199	20000810
AU 2001093720	A5	20020218	AU 2001-93720	20010803
EP 1307229	A1	20030507	EP 2001-974107	20010803

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

PRIORITY APPLN. INFO.: DE 2000-10039199 A 20000810
 WO 2001-EP9008 W 20010803

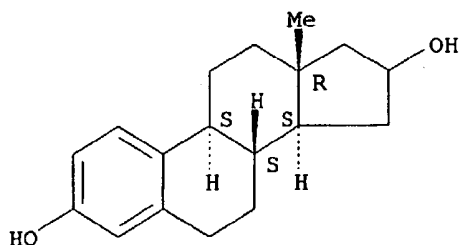
AB A novel medicament for the treatment of estrogen-deficient disease states is disclosed. Said medicament is a combination prepn. comprising an ER.beta.-selective estrogen and an ER.alpha.-selective antiestrogen or SERM (Selective Estrogen Receptor Modulator). The antiestrogen or SERM which is a component of the combination prepn. is preferably selective for the periphery. The prepn. is suitable for an organ-specific estrogen therapy and has clear advantages over conventional therapies. Due to the combination of ER.alpha.-selective SERM and ER.beta.-estrogen the prepn. permits a complete protection against bone loss caused by estrogen deficiency. The components of the medicament also have a synergistic effect with respect to the inhibition of inflammation inducing genes, in particular in inflammatory disorders such as atherosclerosis and arthritis, or neurodegenerative diseases such as Alzheimers and multiple sclerosis. Furthermore, pos. effects on cognition and mood may be expected. The protective estrogen-like effects are achieved, with no expectation of proliferation effects on breasts or uterus.

IT 397872-24-1D, Estra-1,3,5(10)-triene-3,16-diol, derivs.
 RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (combination prepn. with an ER.beta. selective estrogen and a SERM or antiestrogen)

RN 397872-24-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:190285 HCAPLUS

DOCUMENT NUMBER: 134:261332

TITLE: QSAR with electrotopological state atom index.
Part-3a. Receptor binding affinity of estrogens and non-steroidal estrogen analogs

AUTHOR(S): Saha, Achintya; Roy, Kunal; De, Kakali; Sengupta, Chandana

CORPORATE SOURCE: Dep. Chemical Technology, Univ. Calcutta, alcutta, 700 009, India

SOURCE: Journal of the Indian Chemical Society (2001), 78(2), 92-97

CODEN: JICSAH; ISSN: 0019-4522

PUBLISHER: Indian Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Quant. structure activity relationship (QSAR) anal. of estrogens and non-steroidal analogs of estrogen with electrotopol. state atom (ETSA) index has been performed to explore the atoms or fragments of the mols. that are most important for the binding affinity to receptor. The study reveals the importance of Ph ring fragment (C1, C5 and C10 atoms of steroidal estrogen, and C1, C3, C4, C9 and C10 atoms in case of non-steroidal analogs) for receptor binding affinity. The importance of these atoms or fragments is also supported from the literature survey. Thus, the Ph ring constitutes the pharmacophore for receptor binding affinity of estrogen analogs. Hence, diagnostic potential of the ETSA scheme in identifying the atoms or fragments important for activity is revealed from the study.

IT 1090-04-6

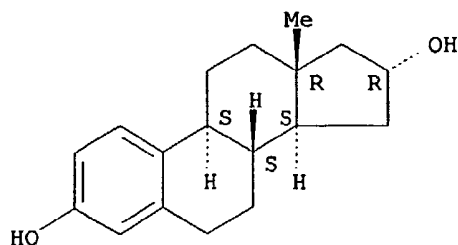
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(QSAR with electrotopol. state atom index in relation to receptor binding affinity of estrogens and non-steroidal estrogen analogs)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:898420 HCAPLUS

DOCUMENT NUMBER: 134:80974

TITLE: A computationally based identification algorithm for estrogen receptor ligands: Part 2. Evaluation of a hER.alpha. binding affinity model

AUTHOR(S): Mekenyan, O. G.; Kamenska, V.; Schmieder, P. K.; Ankley, G. T.; Bradbury, S. P.

CORPORATE SOURCE: Laboratory of Mathematical Chemistry, Department of Physical Chemistry, Bourgas University "Prof. As. Zlatarov.", Bourgas, 118010, Bulg.

SOURCE: Toxicological Sciences (2000), 58(2), 270-281

CODEN: TOSCF2; ISSN: 1096-6080

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The objective of this study was to evaluate the capability of an expert system described in the previous paper to identify the potential for chems. to act as ligands of mammalian estrogen receptors (ERs). The basis of the expert system was a structure activity relationship (SAR) model, based on relative binding affinity (RBA) values for steroidal and nonsteroidal chems. derived from human ER.alpha. (hER.alpha.) competitive binding assays. The expert system enables categorization of chems. into RBA ranges of <0.1, 0.1 to 1, 1 to 10, 10 to 100, and >150% relative to 17.beta.-estradiol. In the current anal., the algorithm was evaluated with respect to predicting RBAs of chems. assayed with ERs from MCF7 cells, and mouse and rat uterine prepns. The best correspondence between predicted and obsd. RBA ranges was obtained with MCF7 cells. The agreement between predictions from the expert system and data from binding assays with mouse and rat ER(s) were less reliable, esp. for chems. with RBAs less than 10%. Prediction errors often were false positives, i.e., predictions of greater than obsd. RBA values. While discrepancies were likely due, in part, to species-specific variations in ER structure and ligand binding affinity, a systematic bias in structural characteristics of chems. in the hER.alpha. training set, compared to the rodent evaluation data sets, also contributed to prediction errors. False-pos. predictions were typically assocd. with ligands that had shielded electroneg. sites. Ligands with these structural characteristics were not well represented in the training set used to derive the expert system. Inclusion of a shielding criterion into the original expert system significantly increased the accuracy of RBA predictions. With this addnl. structural requirement, 38 of 46 compds. with measured RBA values greater than 10% in hER.alpha., MCF7, and rodent uterine prepns. were correctly

categorized. Of the remaining 129 compds. in the combined data sets, RBA values for 65 compds. were correctly predicted, with 47 of the incorrect predictions being false positives. Based upon this exploratory anal., the modeling approach, combined with a high-quality training set of RBA values derived from a diverse set of chem. structures, could provide a credible tool for prioritizing chems. with moderate to high ER binding affinity for subsequent in vitro or in vivo assessments.

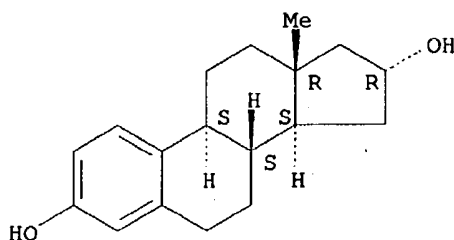
IT 1090-04-6, 16.alpha.-Estradiol

RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(computationally based identification algorithm for estrogen receptor ligand .alpha. binding affinity)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:738805 HCAPLUS

DOCUMENT NUMBER: 133:296594

TITLE: Preparation of ent-steroids as selectively effective estrogens

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19917930	A1	20001019	DE 1999-19917930	19990415
WO 2000063228	A1	20001026	WO 2000-EP3470	20000417
<p>W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM</p> <p>RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG</p>				

EP 1169336 A1 20020109 EP 2000-925219 20000417
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO

JP 2002542255 T2 20021210 JP 2000-612318 20000417
 PRIORITY APPLN. INFO.: DE 1999-19917930 A 19990415
 WO 2000-EP3470 W 20000417

OTHER SOURCE(S): MARPAT 133:296594

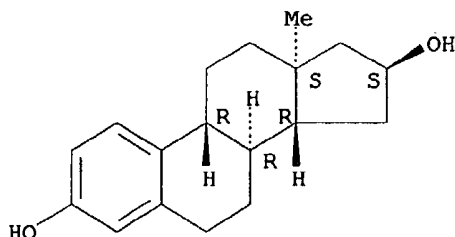
AB The invention describes new ent-steroids I [R1 = H, OR12, alkenyloxy, alkynyloxy, OSO2R13; R2 = OR12, OSO2R13, OC(:O)R16; R3, R4, R5, R8, R9 = H, halogen, OR12, OSO2R13, R16; R6 = .beta.-H; R7 = H; R6R7 = .alpha.-, .beta.-CH2; R10 = H2, dihalogen, H and a halogen, :CR17R18; R11 = H, Me, Et; R12 = H, C1-5-alkyl, C1-5-alkenyl; R13 = , NR14R15; R14, R15 = H, C1-5-alkyl, COR16, C3-7-cycloalkyl, aryl; R14R15 = polymethylene; NR14R15 = morpholine; R16 = C1-12-alkyl, C1-12-alkenyl, C1-12-alkynyl; R17, R18 = H, halogen, H and OR12, H and OSO2R13, R12 and OC(:O)R16, O; one or more double bonds at C(6)-C(7), C(7)-C(8), C(8)-C(9), C(9)-C(11), C(11)-C(12), C(8)-C(14), C(14)-C(15), C(15)-C(16), C(16)-C(17)], as pharmaceutically active substances, which exhibit in vitro a higher affinity at estrogen receptor of rat prostate than at estrogen receptor of Rat uterus and in vivo a preferential effect at the bone in the comparison to the uterus, their prodn., its therapeutic application and pharmaceutical compns., which contain the new compds. Thus, ent-estriol (I; R1 = R3 = R4 = R5 = R6 = R7 = R8 = H, R2 = OH, R9 = .alpha.-OH, R10 = .beta.-OH, R11 = Me) was prepd. stereoselectively from ent-3,16.alpha.-dihydroxyestra-1,3,5(10)-trien-17-one (I; R1 = R3 = R4 = R5 = R6 = R7 = R8 = H, R2 = OH, R9 = .alpha.-OH, R10 = O, R11 = Me) via redn. with NaBH4 in MeOH. Furthermore the invention describes the use of steroids, those with the (8.alpha.-H,9.beta.-H,10.alpha.-H,13.alpha.-H,14.beta.-H)-gonane skeleton, for the treatment of estrogen deficiency conditioned diseases and conditions.

IT 300853-08-1P, ent-Estra-1,3,5(10)-triene-3,16.alpha.-diol
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of ent-steroids as selectively effective estrogens)

RN 300853-08-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (8.alpha.,9.beta.,13.alpha.,14.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:552017 HCAPLUS

DOCUMENT NUMBER: 133:150782

TITLE: synthesis of 16-Hydroxyestratrienes as selectively

effective estrogens
 INVENTOR(S): Kuenzer, Hermann; Knauthe, Rudolf; Lessl, Monika;
 Fritzemeier, Karl-heinrich; Hegele-Hartung, Christa;
 Boemer, Ulf; Mueller, Gerd; Kosemund, Dirk
 PATENT ASSIGNEE(S): Schering A.-G., Germany
 SOURCE: Ger. Offen., 34 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19906159	A1	20000810	DE 1999-19906159	19990209
CA 2359660	AA	20000817	CA 2000-2359660	20000209
WO 2000047603	A2	20000817	WO 2000-EP1073	20000209
WO 2000047603	A3	20010802		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2000029095	A5	20000829	AU 2000-29095	20000209
EP 1144431	A2	20011017	EP 2000-907539	20000209
EP 1144431	A3	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008076	A	20020205	BR 2000-8076	20000209
JP 2002536455	T2	20021029	JP 2000-598520	20000209
EE 200100412	A	20021216	EE 2001-412	20000209
NO 2001003860	A	20011008	NO 2001-3860	20010808
BG 105804	A	20020329	BG 2001-105804	20010809
PRIORITY APPLN. INFO.:			DE 1999-19906159 A	19990209
			WO 2000-EP1073 W	20000209

OTHER SOURCE(S): MARPAT 133:150782

AB Synthesis of 16-Hydroxyestratrienes (I) [R1 = halogen, HO, Me, F3C, MeO, EtO, H; R2 = halogen, HO, (un)substituted alkoxy, H; R4 = halogen, fluoroalkyl, F3C, F5C2, (un)substituted alkoxy, H; R7 = halogen, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkoxy, (un)substituted heteroaryl, (un)substituted aryl, H; R8 = H, fluoroalkyl, fluoroalkenyl, CN; R9 = H, Me, Et, F3C, F5C2; R11 = NO2O, HO, HS, halogen, chloromethyl, fluoroalkenyl, fluoroalkyl, (un)substituted alkoxy, (un)substituted alkylthio, (un)substituted aryl, (un)substituted heteroaryl, H; R13 = Me, Et, F3C, F5C2; R14 = (un)substituted alkenyl, (un)substituted alkyl, H; R15 = halogen, fluoroalkyl, fluoroalkenyl, =O, =S, SO, SO2, (un)substituted =NH; R14, R15 together = methylene; R16 = fluoroalkyl, fluoroalkenyl, F3C, F5C2, CN, H; R17 = fluoroalkyl, fluoroalkenyl, H, HO] as selectively effective estrogens is disclosed. Thus, 16.alpha.-estradiol shows a 50% uterine stimulation at 30 .upsilon.g in in vivo testing.

IT 287721-55-5P 287721-56-6P 287721-57-7P
 287721-58-8P 287721-59-9P 287721-60-2P

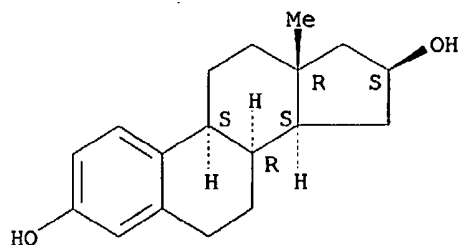
287721-61-3P 287721-62-4P 287721-63-5P
287721-64-6P 287721-66-8P 287721-67-9P
287721-71-5P 287721-72-6P 287721-73-7P
287721-74-8P 287721-75-9P 287721-77-1P
287721-80-6P 287721-81-7P 287721-85-1P
287721-86-2P 287721-87-3P 287721-88-4P
287721-90-8P 287721-93-1P 287721-94-2P
287721-95-3P 287721-96-4P 287721-98-6P
287722-00-3P 287722-01-4P 287722-02-5P
287722-03-6P 287722-04-7P 287722-06-9P
287722-08-1P 287722-09-2P 287722-10-5P
287722-11-6P 287722-12-7P 287722-14-9P
287722-16-1P 287722-17-2P 287722-18-3P
287722-19-4P 287722-20-7P 287722-22-9P
287722-24-1P 287722-25-2P 287722-26-3P
287722-27-4P 287722-28-5P 287722-29-6P
287722-30-9P 287722-31-0P 287722-32-1P
287722-33-2P 287722-34-3P 287722-35-4P
287722-36-5P 287722-37-6P 287722-38-7P
287722-39-8P 287722-40-1P 287722-41-2P
287722-42-3P 287722-43-4P 287722-44-5P
287722-45-6P 287722-46-7P 287722-47-8P
287722-48-9P 287722-49-0P 287722-50-3P
287722-51-4P 287722-52-5P 287722-53-6P
287722-54-7P 287722-55-8P 287722-56-9P
287722-57-0P 287722-58-1P 287722-59-2P
287722-60-5P 287722-61-6P 287722-62-7P
287722-64-9P 287722-66-1P 287722-67-2P
287722-68-3P 287722-69-4P 287722-70-7P
287722-72-9P 287722-74-1P 287722-75-2P
287722-76-3P 287722-77-4P 287722-78-5P
287722-80-9P 287722-82-1P 287722-83-2P
287722-84-3P 287722-85-4P 287722-86-5P
287722-88-7P 287722-90-1P 287722-91-2P
287722-92-3P 287722-93-4P 287722-94-5P
287722-95-6P 287722-96-7P 287722-97-8P
287722-98-9P 287722-99-0P 287723-00-6P
287723-01-7P 287723-02-8P 287723-03-9P
287723-04-0P 287723-05-1P 287723-06-2P
287723-07-3P 287723-08-4P 287723-09-5P
287723-10-8P 287723-11-9P 287723-12-0P
287723-13-1P 287723-14-2P 287723-15-3P
287723-16-4P 287723-17-5P 287723-18-6P
287723-19-7P 287723-20-0P 287723-21-1P
287723-22-2P 287724-23-6P 287724-24-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of 16-Hydroxyestratrienes as selectively effective estrogens)

RN 287721-55-5 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, (8.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

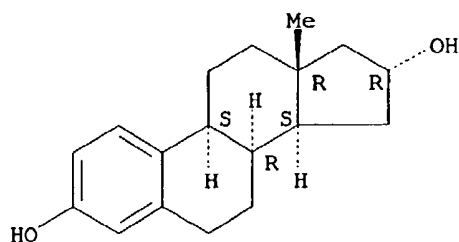
Absolute stereochemistry. Rotation (+).



RN 287721-56-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (8.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

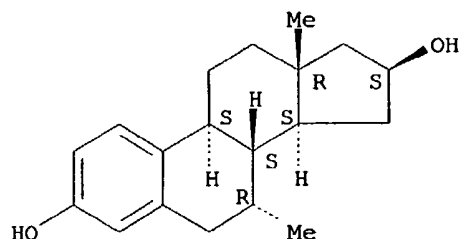
Absolute stereochemistry. Rotation (+).



RN 287721-57-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

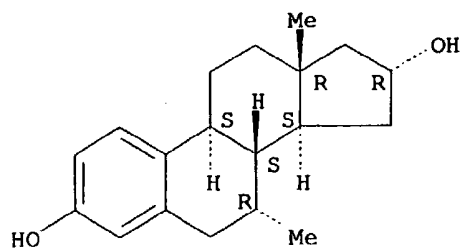
Absolute stereochemistry. Rotation (+).



RN 287721-58-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methyl-, (7.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

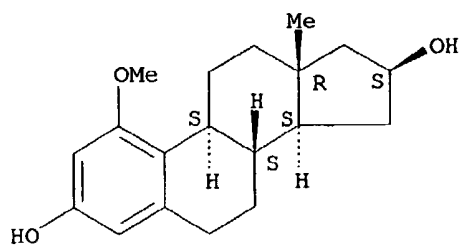
Absolute stereochemistry. Rotation (+).



RN 287721-59-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16.beta.)- (9CI) (CA INDEX NAME)

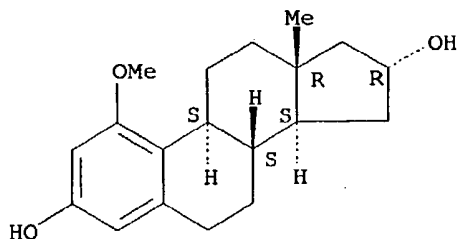
Absolute stereochemistry.



RN 287721-60-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 1-methoxy-, (16.alpha.)- (9CI) (CA INDEX NAME)

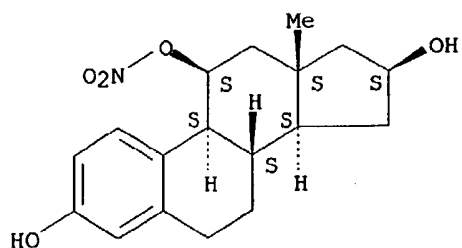
Absolute stereochemistry.



RN 287721-61-3 HCAPLUS

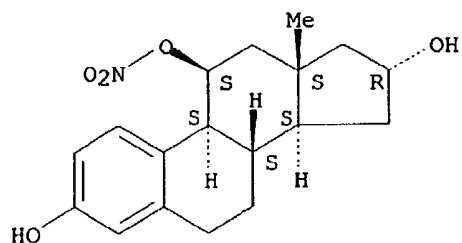
CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate, (11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



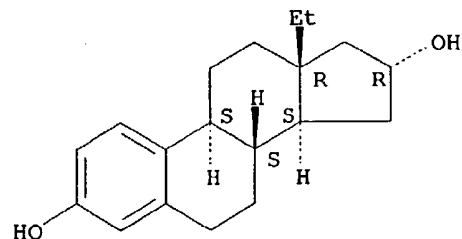
RN 287721-62-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,11,16-triol, 11-nitrate, (11.beta.,16.alpha.)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



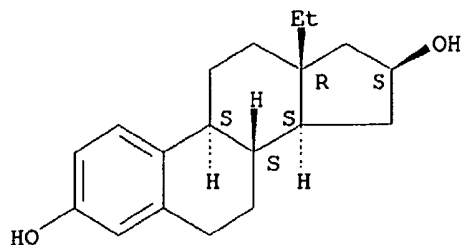
RN 287721-63-5 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16.alpha.)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry. Rotation (+).



RN 287721-64-6 HCAPLUS
 CN Gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-, (16.beta.)- (9CI) (CA INDEX
 NAME)

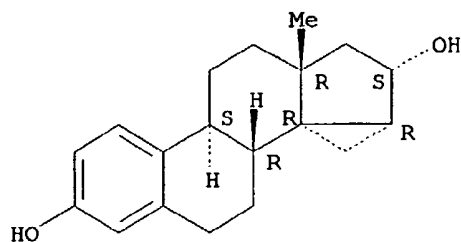
Absolute stereochemistry. Rotation (+).



RN 287721-66-8 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14R,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

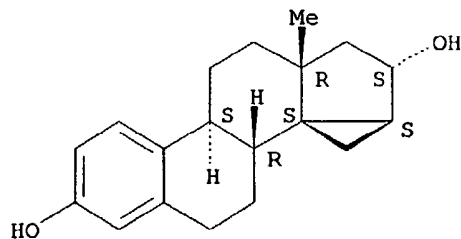
Absolute stereochemistry.



RN 287721-67-9 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14S,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

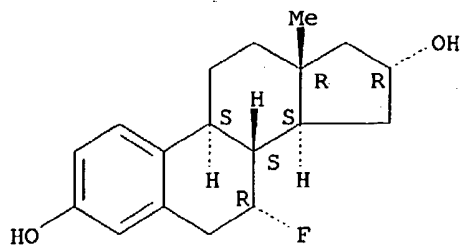
Absolute stereochemistry.



RN 287721-71-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

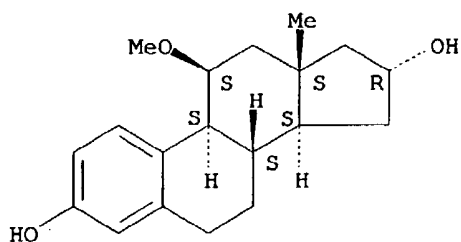
Absolute stereochemistry.



RN 287721-72-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-, (11.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

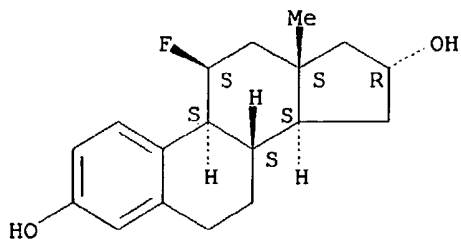
Absolute stereochemistry.



RN 287721-73-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

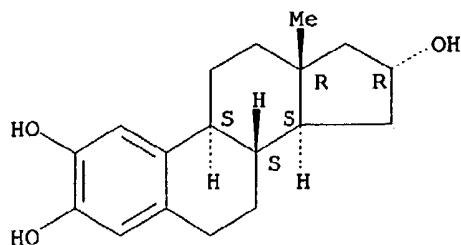
Absolute stereochemistry.



RN 287721-74-8 HCAPLUS

CN Estra-1,3,5(10)-triene-2,3,16-triol, (16.alpha.)- (9CI) (CA INDEX NAME)

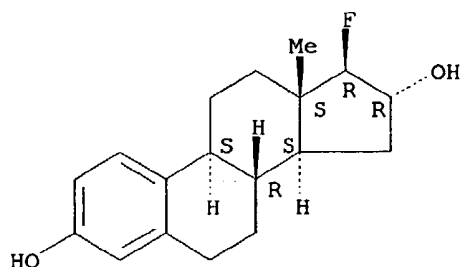
Absolute stereochemistry.



RN 287721-75-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16.alpha.,17.beta.)- (9CI)
(CA INDEX NAME)

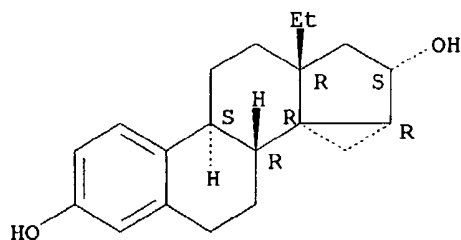
Absolute stereochemistry.



RN 287721-77-1 HCAPLUS

CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-,
(14R,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

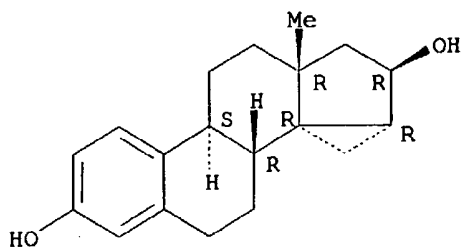
Absolute stereochemistry.



RN 287721-80-6 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14R,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

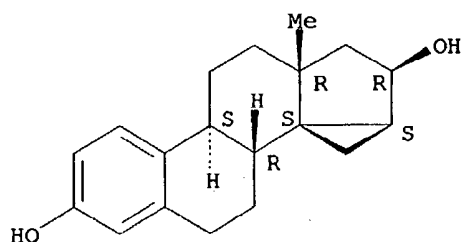
Absolute stereochemistry.



RN 287721-81-7 HCAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-3,16-diol, 3',15-dihydro-,
(14S,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

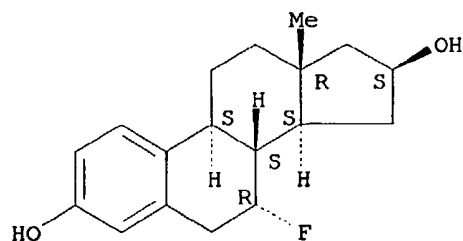
Absolute stereochemistry.



RN 287721-85-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-fluoro-, (7.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

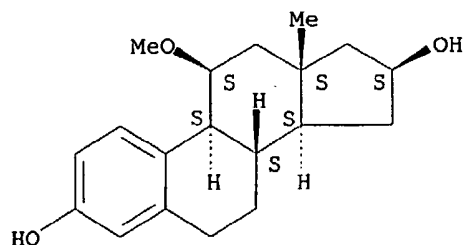
Absolute stereochemistry.



RN 287721-86-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-methoxy-, (11.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

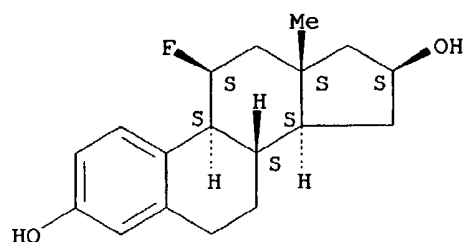
Absolute stereochemistry.



RN 287721-87-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-, (11.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

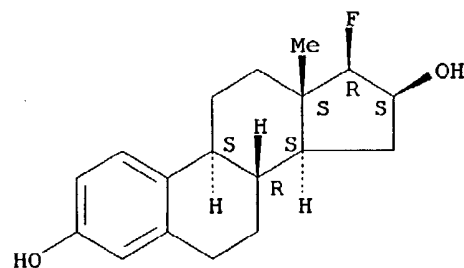
Absolute stereochemistry.



RN 287721-88-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 17-fluoro-, (16.beta.,17.beta.)- (9CI)
(CA INDEX NAME)

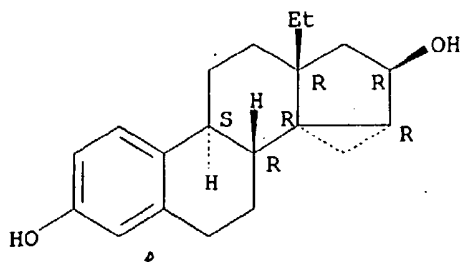
Absolute stereochemistry.



RN 287721-90-8 HCAPLUS

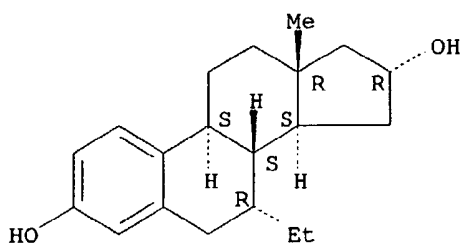
CN Cyclopropa[14,15]gona-1,3,5(10)-triene-3,16-diol, 13-ethyl-3',15-dihydro-,
(14R,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



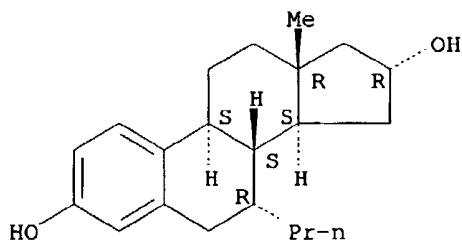
RN 287721-93-1 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7.alpha.,16.alpha.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



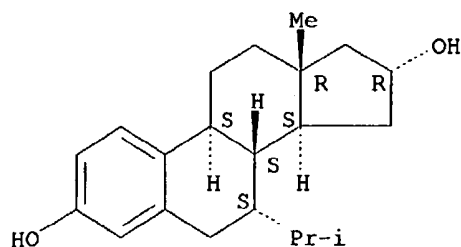
RN 287721-94-2 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7.alpha.,16.alpha.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 287721-95-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.alpha.,16.alpha.)-
 (9CI) (CA INDEX NAME)

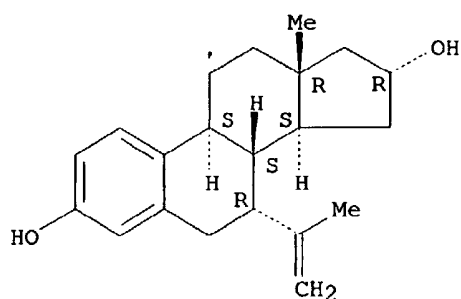
Absolute stereochemistry.



RN 287721-96-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

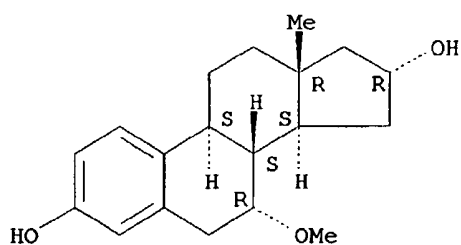
Absolute stereochemistry.



RN 287721-98-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

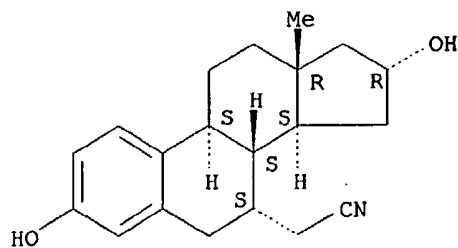
Absolute stereochemistry.



RN 287722-00-3 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

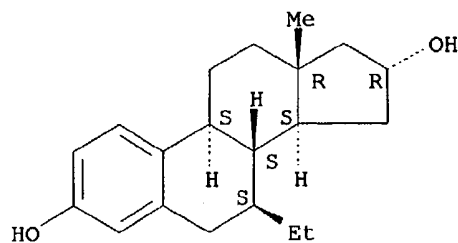
Absolute stereochemistry.



RN 287722-01-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

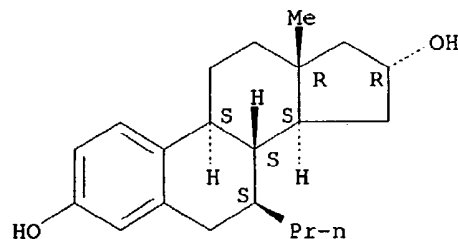
Absolute stereochemistry.



RN 287722-02-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

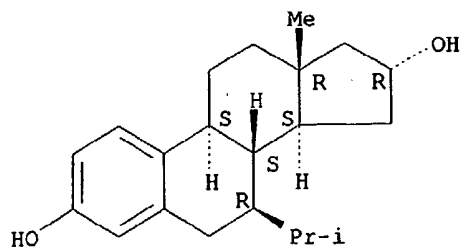
Absolute stereochemistry.



RN 287722-03-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.beta.,16.alpha.)-
(9CI) (CA INDEX NAME)

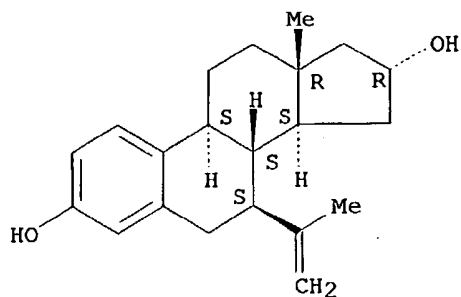
Absolute stereochemistry.



RN 287722-04-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethenyl)-,
(7.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

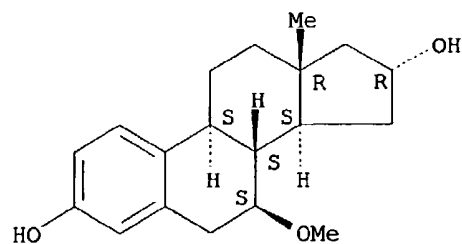
Absolute stereochemistry.



RN 287722-06-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-methoxy-, (7.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

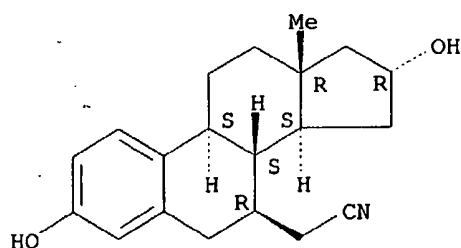
Absolute stereochemistry.



RN 287722-08-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 3,16-dihydroxy-,
(7.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

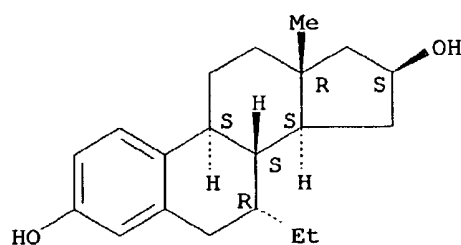
Absolute stereochemistry.



RN 287722-09-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

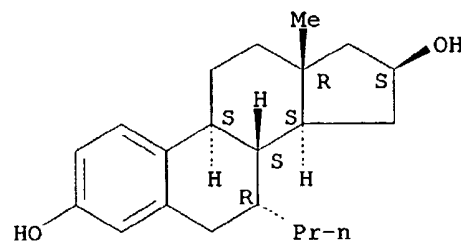
Absolute stereochemistry.



RN 287722-10-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

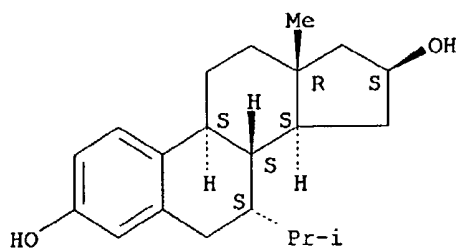
Absolute stereochemistry.



RN 287722-11-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.alpha.,16.beta.)-
(9CI) (CA INDEX NAME)

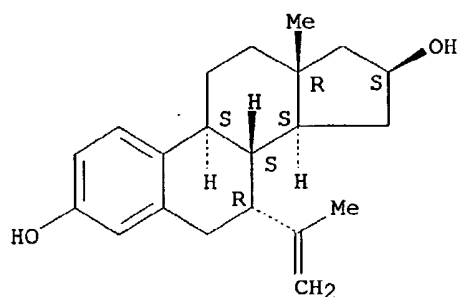
Absolute stereochemistry.



RN 287722-12-7 HCAPLUS

CN Estradiol, 17β-hydroxy-, 17α-(1-methylethenyl)-, (17α,20β)- (9CI) (CA INDEX NAME)

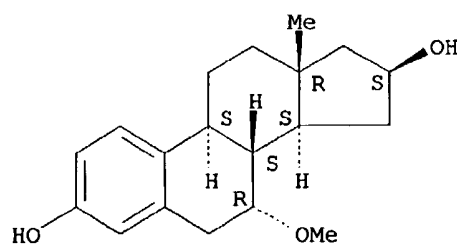
Absolute stereochemistry.



RN 287722-14-9 HCAPLUS

CN Estrone, 17-ketone-, 17α-(1-methylethenyl)-, (17α,20β)- (9CI) (CA INDEX NAME)

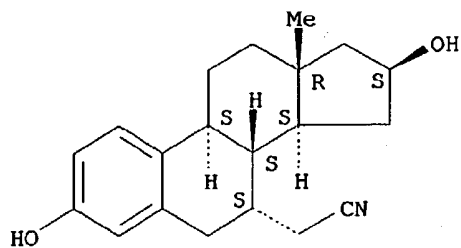
Absolute stereochemistry.



RN 287722-16-1 HCAPLUS

CN Estrone, 17-ketone-, 17α-(1-methylethenyl)-, (17α,20β)- (9CI) (CA INDEX NAME)

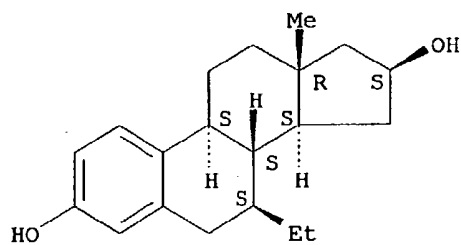
Absolute stereochemistry.



RN 287722-17-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-, (7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

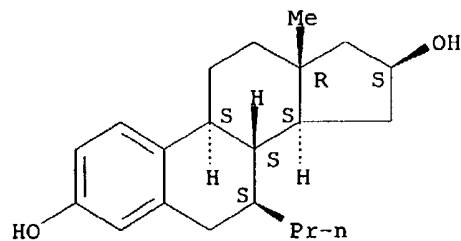
Absolute stereochemistry.



RN 287722-18-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-propyl-, (7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

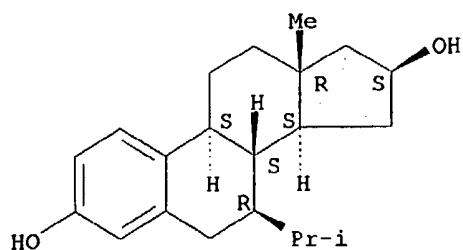
Absolute stereochemistry.



RN 287722-19-4 HCAPLUS

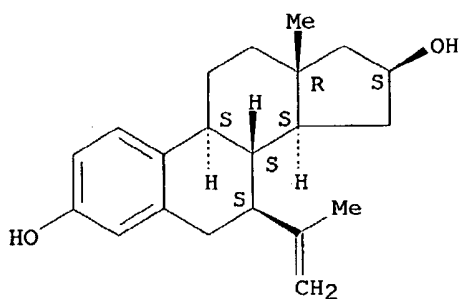
CN Estra-1,3,5(10)-triene-3,16-diol, 7-(1-methylethyl)-, (7.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



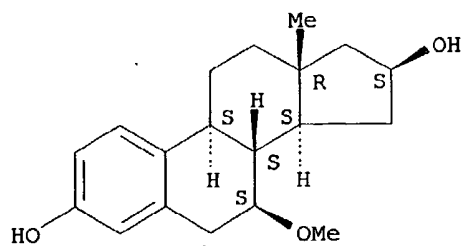
RN 287722-20-7 HCAPLUS
 CN Estradiol, 7-(1-methylethenyl)-, (7.β.,16.β.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



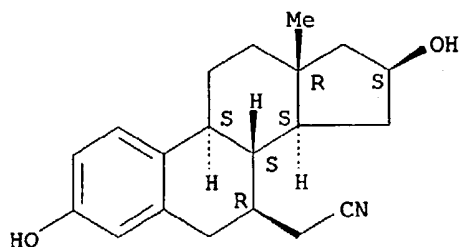
RN 287722-22-9 HCAPLUS
 CN Estrone, 7-methoxy-, (7.β.,16.β.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-24-1 HCAPLUS
 CN Estrone, 7-acetonitrile, 3,16-dihydroxy-, (7.β.,16.β.)- (9CI) (CA INDEX NAME)

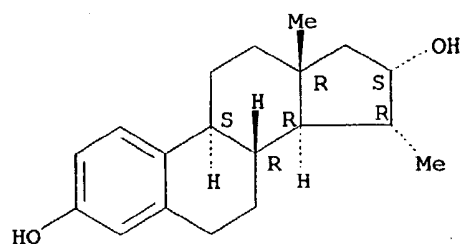
Absolute stereochemistry.



RN 287722-25-2 HCAPLUS

CN Estradiol, 17-cyano-15-methyl-, (15.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

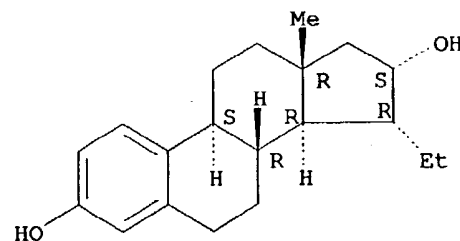
Absolute stereochemistry.



RN 287722-26-3 HCAPLUS

CN Estradiol, 17-ethyl-15-methyl-, (15.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

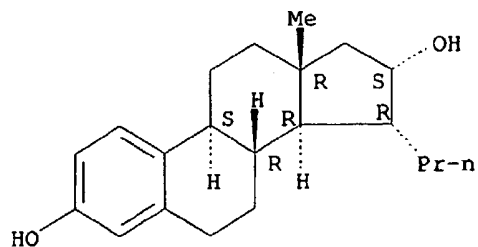
Absolute stereochemistry.



RN 287722-27-4 HCAPLUS

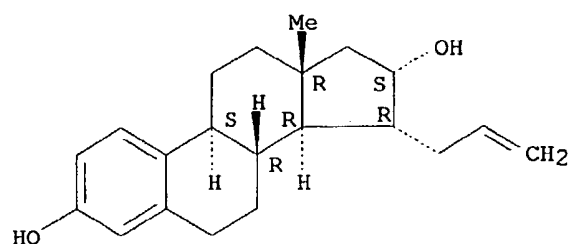
CN Estradiol, 17-propyl-15-methyl-, (15.alpha.,16.alpha.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



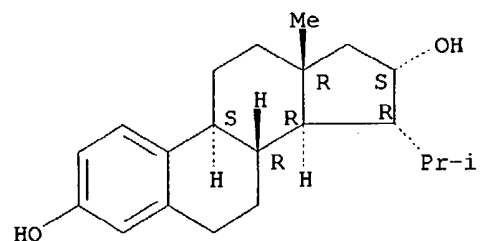
RN 287722-28-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15.alpha.,16.alpha.)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



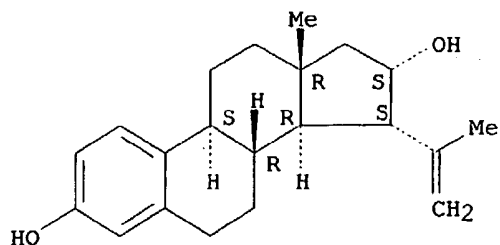
RN 287722-29-6 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
 (15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-30-9 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
 (15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

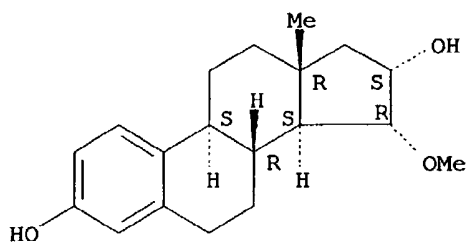
Absolute stereochemistry.



RN 287722-31-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15.alpha.,16.alpha.)-
(9CI) (CA INDEX NAME)

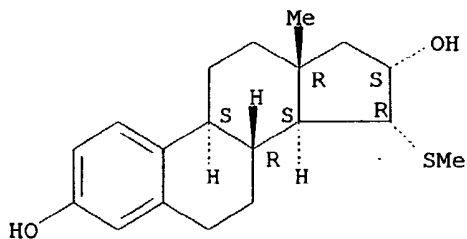
Absolute stereochemistry.



RN 287722-32-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15.alpha.,16.alpha.)-
(9CI) (CA INDEX NAME)

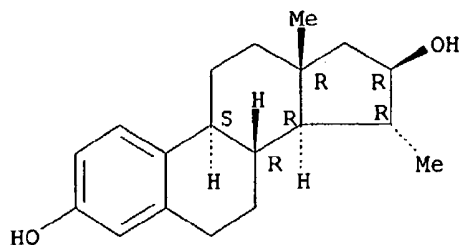
Absolute stereochemistry.



RN 287722-33-2 HCAPLUS

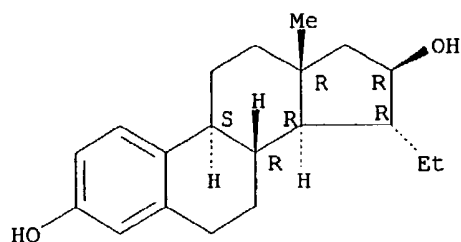
CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



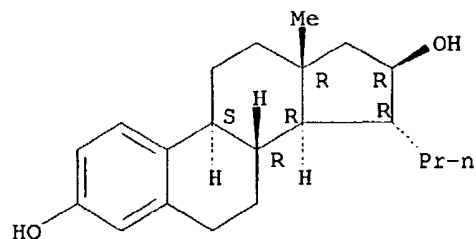
RN 287722-34-3 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15.alpha.,16.beta.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



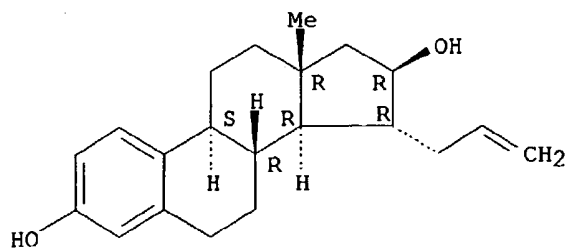
RN 287722-35-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15.alpha.,16.beta.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



RN 287722-36-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15.alpha.,16.beta.)-
 (9CI) (CA INDEX NAME)

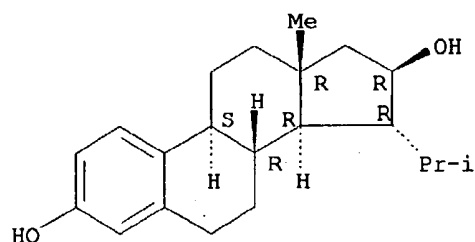
Absolute stereochemistry.



RN 287722-37-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

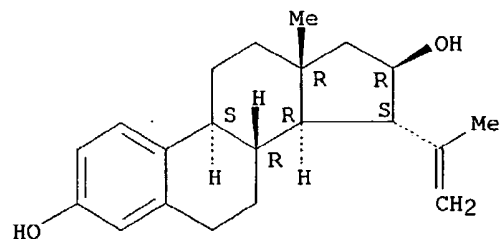
Absolute stereochemistry.



RN 287722-38-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

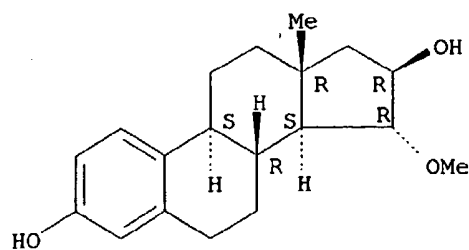
Absolute stereochemistry.



RN 287722-39-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15.alpha.,16.beta.)- (9CI)
(CA INDEX NAME)

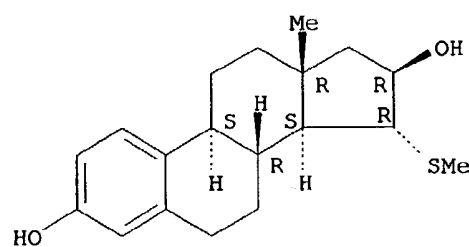
Absolute stereochemistry.



RN 287722-40-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15.alpha.,16.beta.)-
(9CI) (CA INDEX NAME)

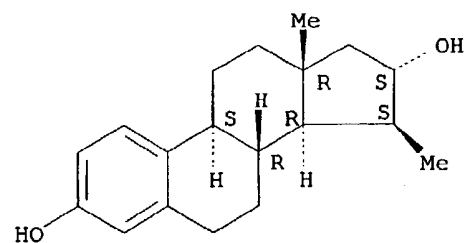
Absolute stereochemistry.



RN 287722-41-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

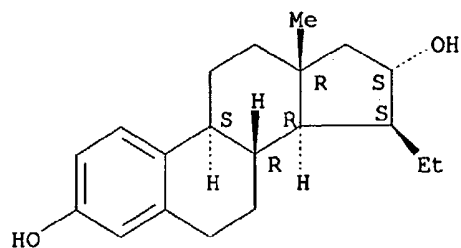
Absolute stereochemistry.



RN 287722-42-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

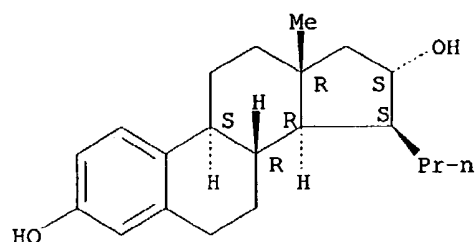
Absolute stereochemistry.



RN 287722-43-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

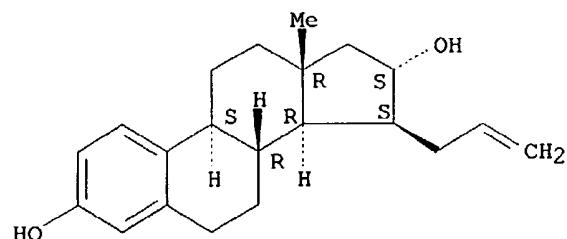
Absolute stereochemistry.



RN 287722-44-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15.beta.,16.alpha.)-
(9CI) (CA INDEX NAME)

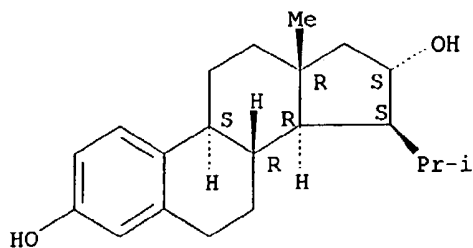
Absolute stereochemistry.



RN 287722-45-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

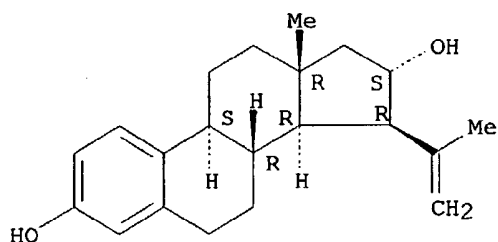
Absolute stereochemistry.



RN 287722-46-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

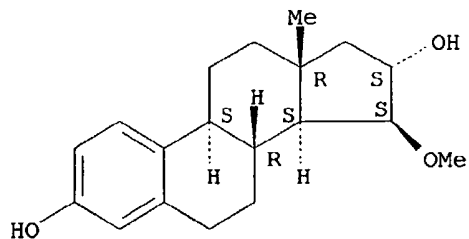
Absolute stereochemistry.



RN 287722-47-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15.beta.,16.alpha.)- (9CI)
(CA INDEX NAME)

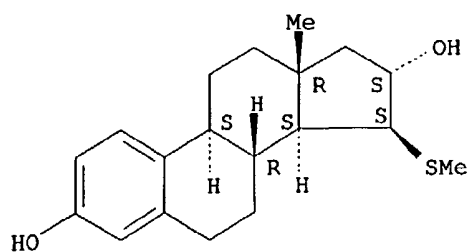
Absolute stereochemistry.



RN 287722-48-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15.beta.,16.alpha.)-
(9CI) (CA INDEX NAME)

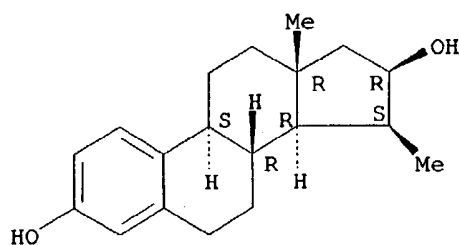
Absolute stereochemistry.



RN 287722-49-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methyl-, (15.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

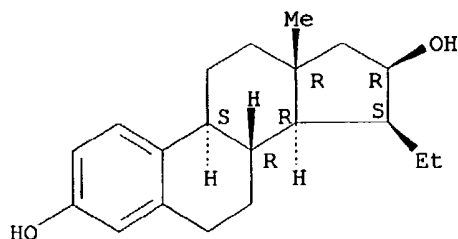
Absolute stereochemistry.



RN 287722-50-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-, (15.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

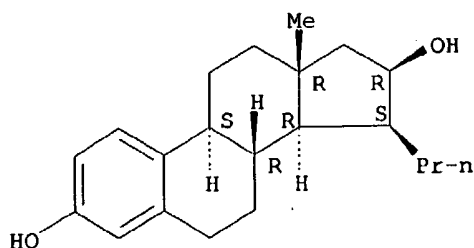
Absolute stereochemistry.



RN 287722-51-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-propyl-, (15.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

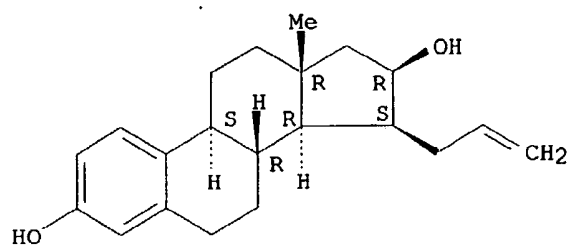
Absolute stereochemistry.



RN 287722-52-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(2-propenyl)-, (15.beta.,16.beta.)-
(9CI) (CA INDEX NAME)

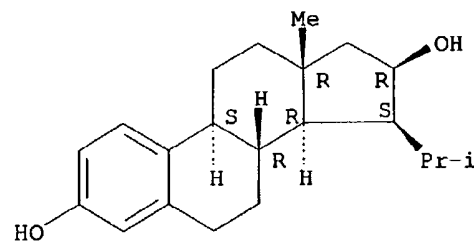
Absolute stereochemistry.



RN 287722-53-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethyl)-,
(15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

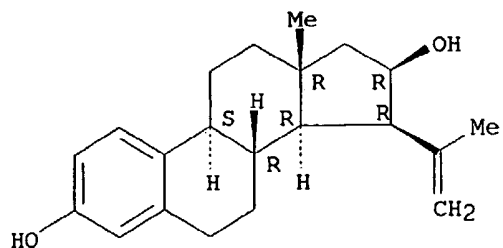
Absolute stereochemistry.



RN 287722-54-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(1-methylethenyl)-,
(15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

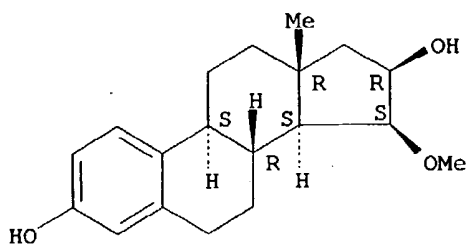
Absolute stereochemistry.



RN 287722-55-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-methoxy-, (15.beta.,16.beta.)- (9CI)
(CA INDEX NAME)

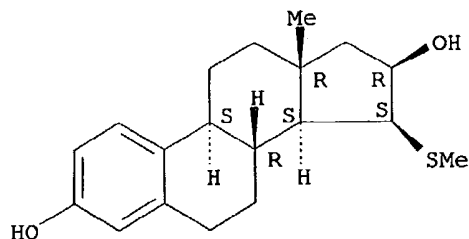
Absolute stereochemistry.



RN 287722-56-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-(methylthio)-, (15.beta.,16.beta.)-
(9CI) (CA INDEX NAME)

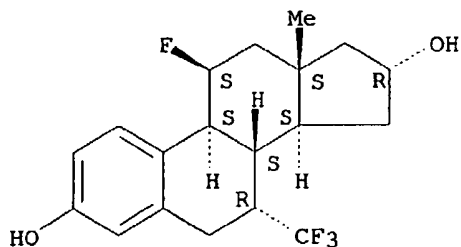
Absolute stereochemistry.



RN 287722-57-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(trifluoromethyl)-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

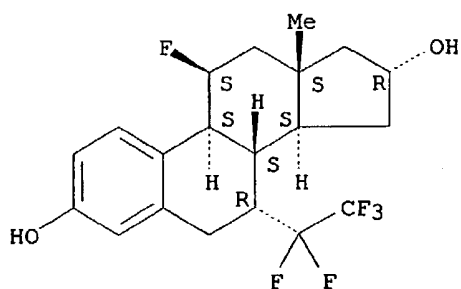
Absolute stereochemistry.



RN 287722-58-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(pentafluoroethyl)-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

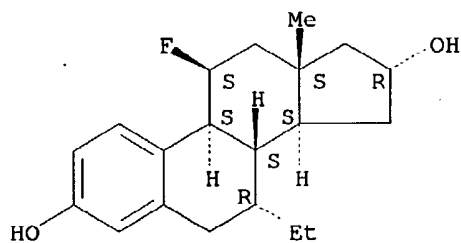
Absolute stereochemistry.



RN 287722-59-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

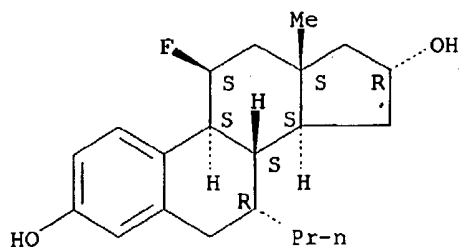
Absolute stereochemistry.



RN 287722-60-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

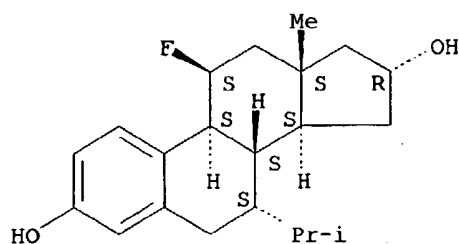
Absolute stereochemistry.



RN 287722-61-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

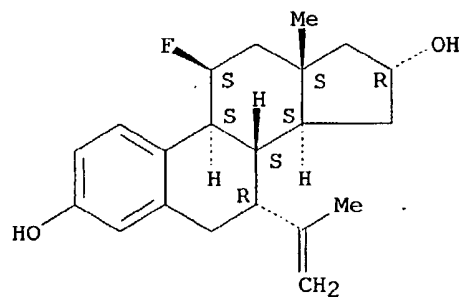
Absolute stereochemistry.



RN 287722-62-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

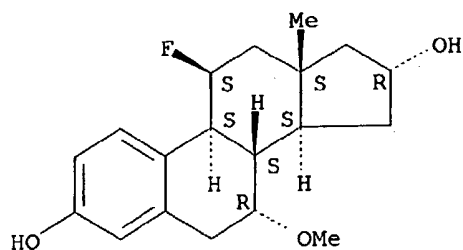
Absolute stereochemistry.



RN 287722-64-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

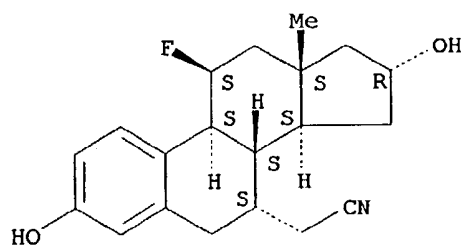
Absolute stereochemistry.



RN 287722-66-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7.alpha.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

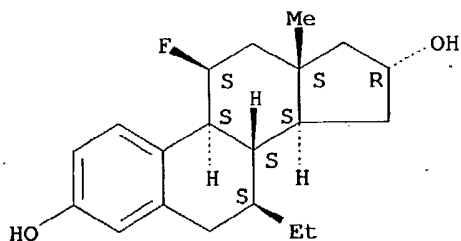
Absolute stereochemistry.



RN 287722-67-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7.beta.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

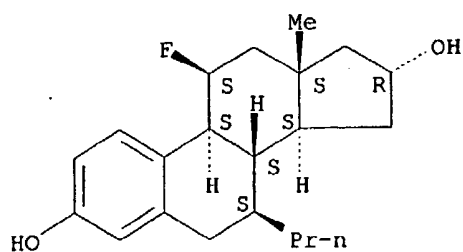
Absolute stereochemistry.



RN 287722-68-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7.beta.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

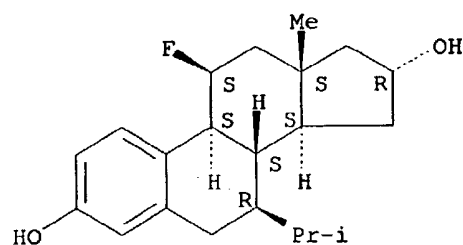
Absolute stereochemistry.



RN 287722-69-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.β.,11.β.,16.α.)- (9CI) (CA INDEX NAME)

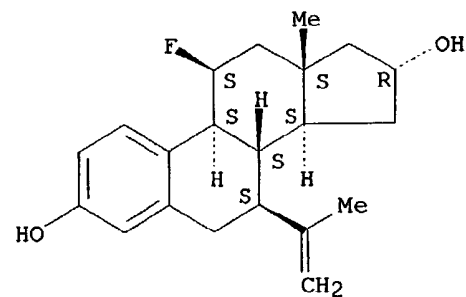
Absolute stereochemistry.



RN 287722-70-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.β.,11.β.,16.α.)- (9CI) (CA INDEX NAME)

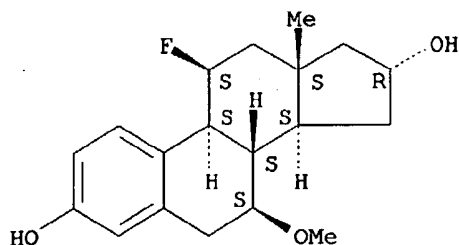
Absolute stereochemistry.



RN 287722-72-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.β.,11.β.,16.α.)- (9CI) (CA INDEX NAME)

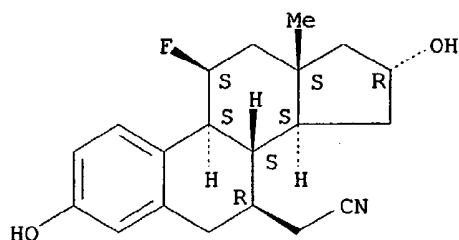
Absolute stereochemistry.



RN 287722-74-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7.beta.,11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

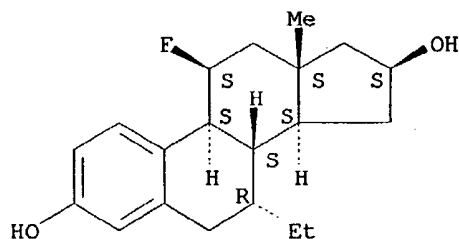
Absolute stereochemistry.



RN 287722-75-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

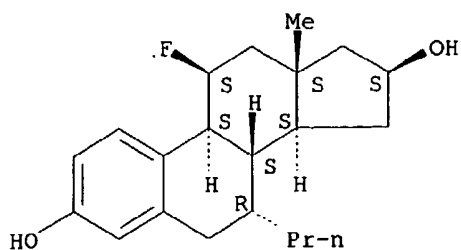
Absolute stereochemistry.



RN 287722-76-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

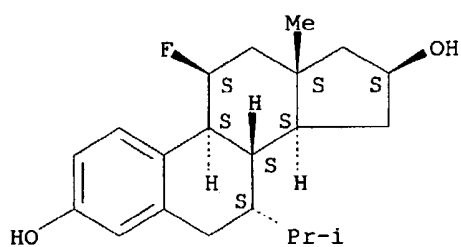
Absolute stereochemistry.



RN 287722-77-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

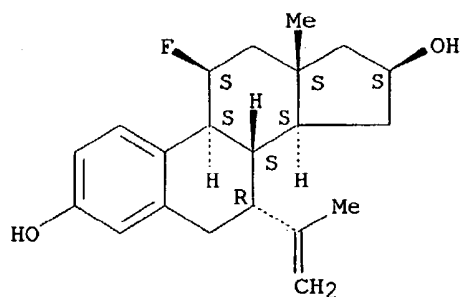
Absolute stereochemistry.



RN 287722-78-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

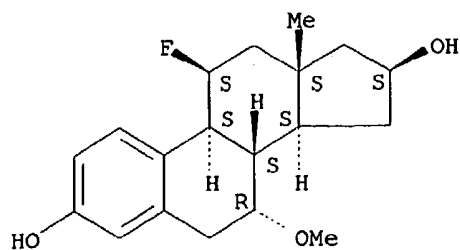
Absolute stereochemistry.



RN 287722-80-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

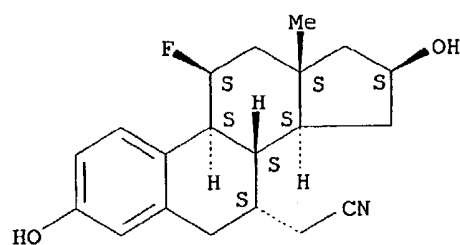
Absolute stereochemistry.



RN 287722-82-1 HCAPLUS

CN Estradiol-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7.alpha.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

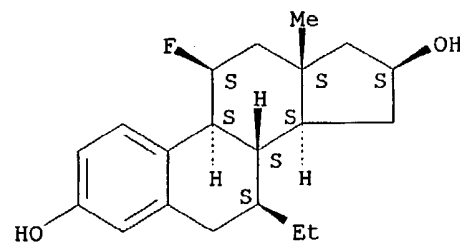
Absolute stereochemistry.



RN 287722-83-2 HCAPLUS

CN Estradiol-1,3,5(10)-triene-3,16-diol, 7-ethyl-11-fluoro-,
(7.beta.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

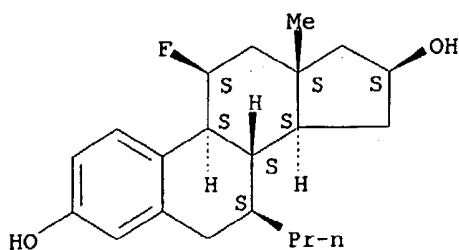
Absolute stereochemistry.



RN 287722-84-3 HCAPLUS

CN Estradiol-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-propyl-,
(7.beta.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

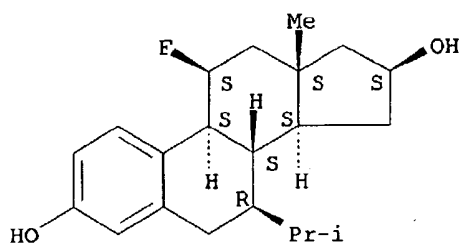
Absolute stereochemistry.



RN 287722-85-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethyl)-,
(7.β.,11.β.,16.β.)- (9CI) (CA INDEX NAME)

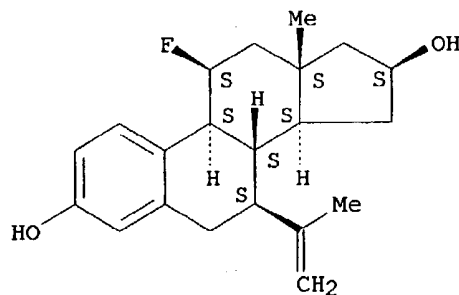
Absolute stereochemistry.



RN 287722-86-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-(1-methylethenyl)-,
(7.β.,11.β.,16.β.)- (9CI) (CA INDEX NAME)

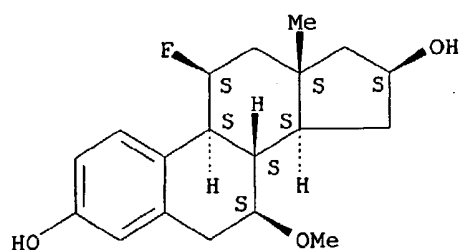
Absolute stereochemistry.



RN 287722-88-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-7-methoxy-,
(7.β.,11.β.,16.β.)- (9CI) (CA INDEX NAME)

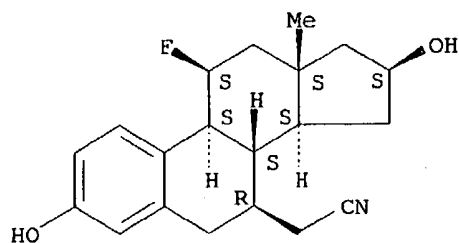
Absolute stereochemistry.



RN 287722-90-1 HCAPLUS

CN Estra-1,3,5(10)-triene-7-acetonitrile, 11-fluoro-3,16-dihydroxy-,
(7.beta.,11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

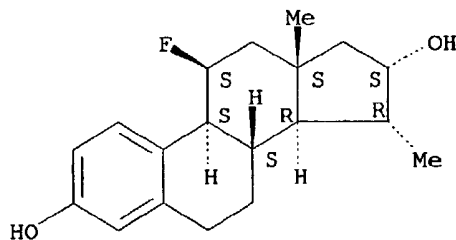
Absolute stereochemistry.



RN 287722-91-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

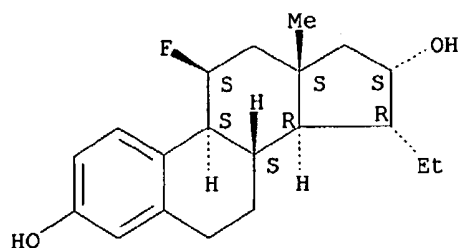
Absolute stereochemistry.



RN 287722-92-3 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

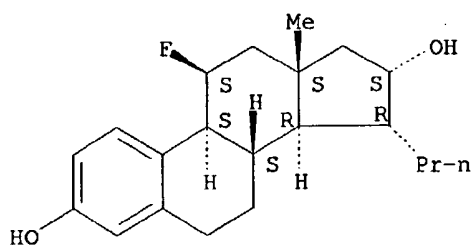
Absolute stereochemistry.



RN 287722-93-4 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

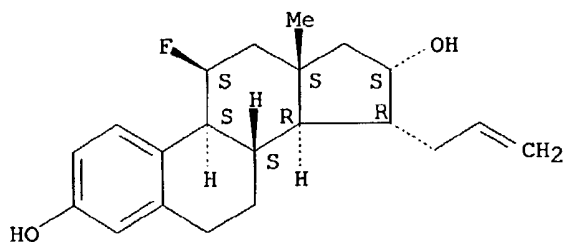
Absolute stereochemistry.



RN 287722-94-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

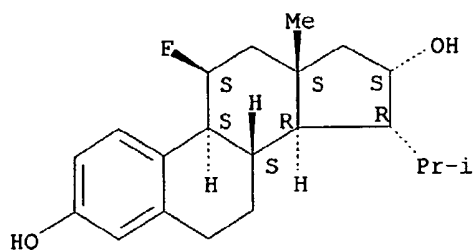
Absolute stereochemistry.



RN 287722-95-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

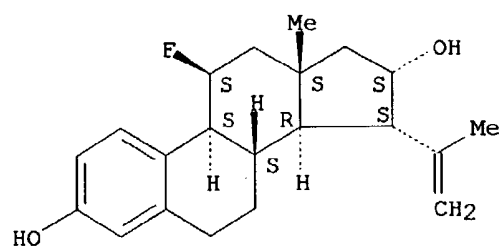
Absolute stereochemistry.



RN 287722-96-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

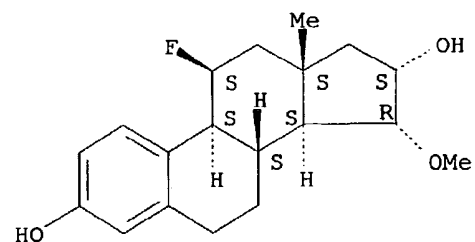
Absolute stereochemistry.



RN 287722-97-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

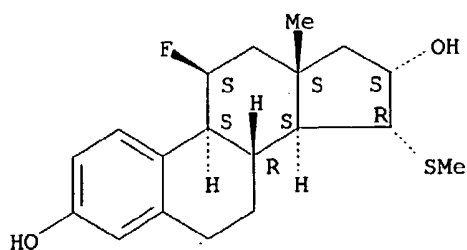
Absolute stereochemistry.



RN 287722-98-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
(11.beta.,15.alpha.,16.alpha.)- (9CI) (CA INDEX NAME)

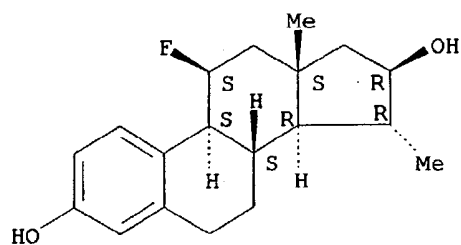
Absolute stereochemistry.



RN 287722-99-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methyl-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

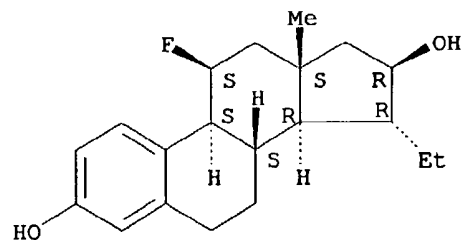
Absolute stereochemistry.



RN 287723-00-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

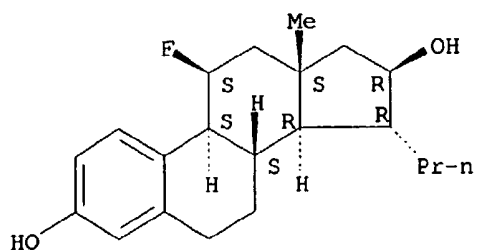
Absolute stereochemistry.



RN 287723-01-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

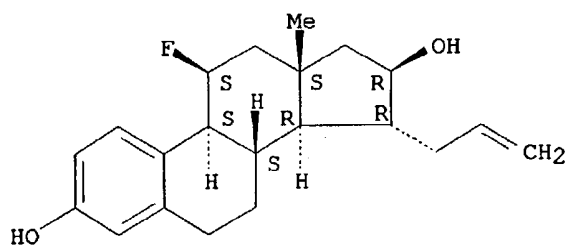
Absolute stereochemistry.



RN 287723-02-8 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

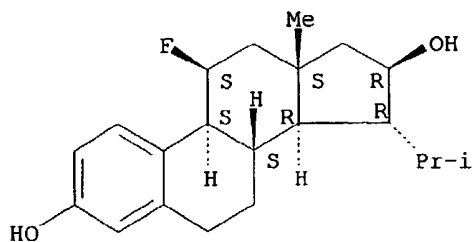
Absolute stereochemistry.



RN 287723-03-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

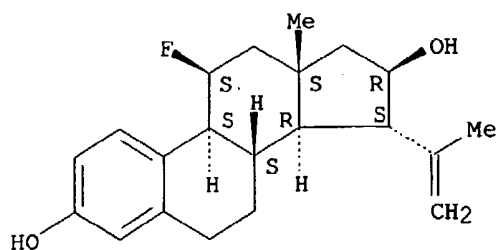
Absolute stereochemistry.



RN 287723-04-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

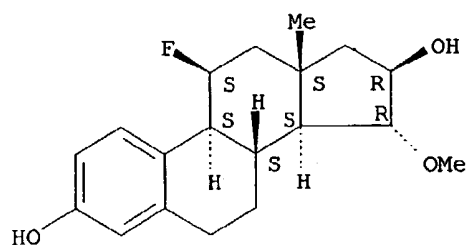
Absolute stereochemistry.



RN 287723-05-1 HCAPLUS

CN Estradiol, 11-fluoro-15-methoxy-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

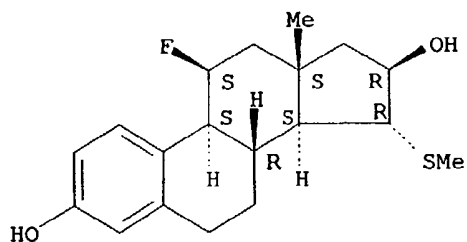
Absolute stereochemistry.



RN 287723-06-2 HCAPLUS

CN Estradiol, 11-fluoro-15-(methylthio)-,
(11.beta.,15.alpha.,16.beta.)- (9CI) (CA INDEX NAME)

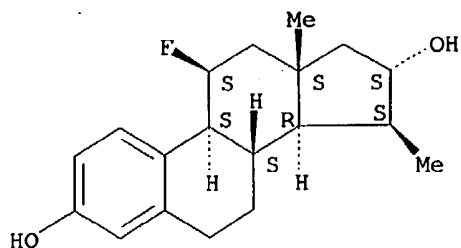
Absolute stereochemistry.



RN 287723-07-3 HCAPLUS

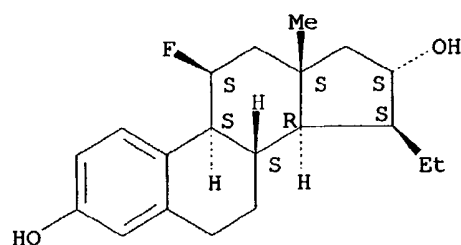
CN Estradiol, 11-fluoro-15-methyl-,
(11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



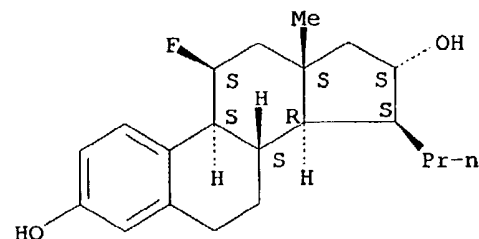
RN 287723-08-4 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 15-ethyl-11-fluoro-,
 (11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



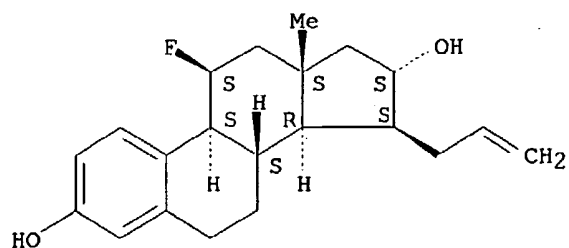
RN 287723-09-5 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
 (11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 287723-10-8 HCAPLUS
 CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
 (11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

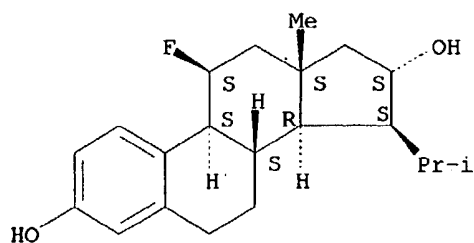
Absolute stereochemistry.



RN 287723-11-9 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

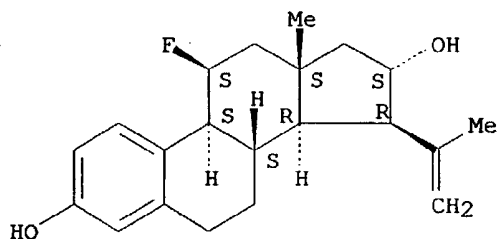
Absolute stereochemistry.



RN 287723-12-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

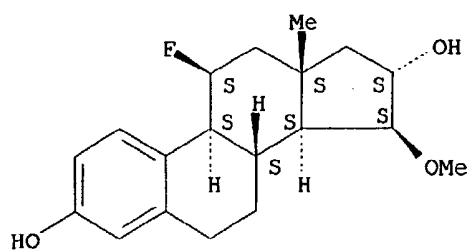
Absolute stereochemistry.



RN 287723-13-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
(11.beta.,15.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

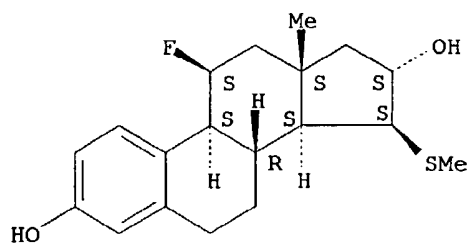
Absolute stereochemistry.



RN 287723-14-2 HCAPLUS

CN Estradiol, 11-fluoro-15-(methylthio)-, (11.β.,15.β.,16.α.)- (9CI) (CA INDEX NAME)

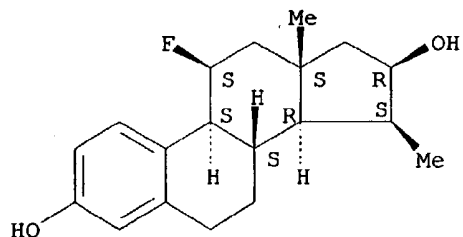
Absolute stereochemistry.



RN 287723-15-3 HCAPLUS

CN Estradiol, 11-fluoro-15-methyl-, (11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

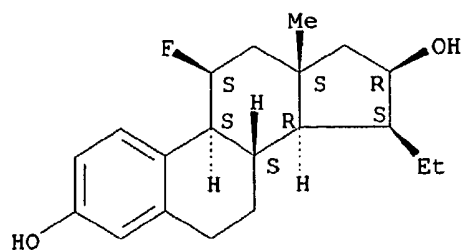
Absolute stereochemistry.



RN 287723-16-4 HCAPLUS

CN Estradiol, 15-ethyl-11-fluoro-, (11.β.,15.β.,16.β.)- (9CI) (CA INDEX NAME)

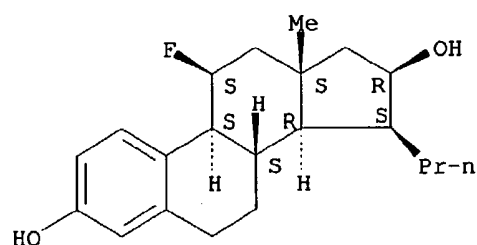
Absolute stereochemistry.



RN 287723-17-5 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-propyl-,
(11.beta.,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

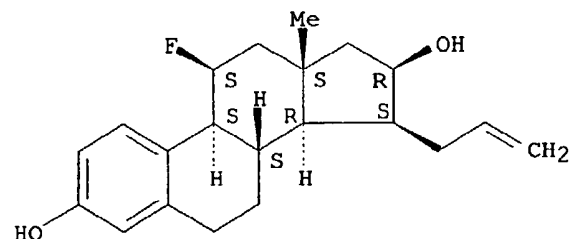
Absolute stereochemistry.



RN 287723-18-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(2-propenyl)-,
(11.beta.,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

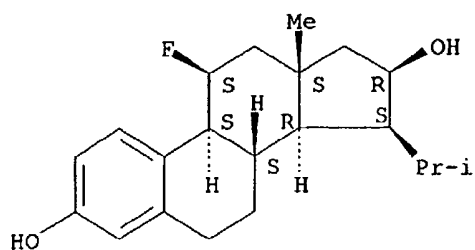
Absolute stereochemistry.



RN 287723-19-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethyl)-,
(11.beta.,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

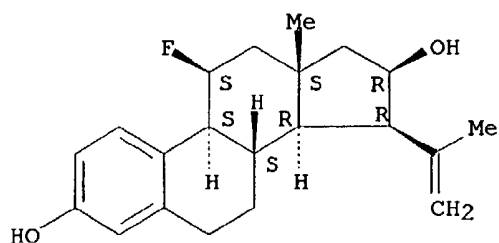
Absolute stereochemistry.



RN 287723-20-0 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(1-methylethenyl)-,
(11.beta.,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

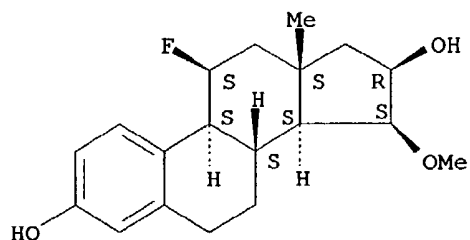
Absolute stereochemistry.



RN 287723-21-1 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-methoxy-,
(11.beta.,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

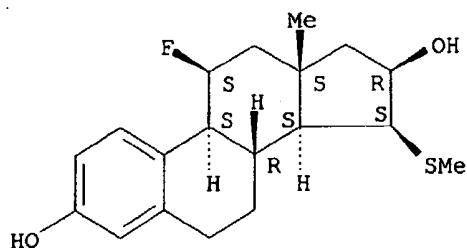
Absolute stereochemistry.



RN 287723-22-2 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-fluoro-15-(methylthio)-,
(11.beta.,15.beta.,16.beta.)- (9CI) (CA INDEX NAME)

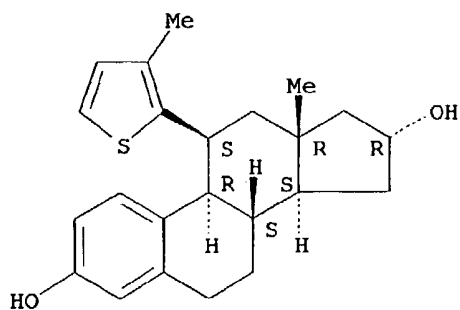
Absolute stereochemistry.



RN 287724-23-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-,
(11.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

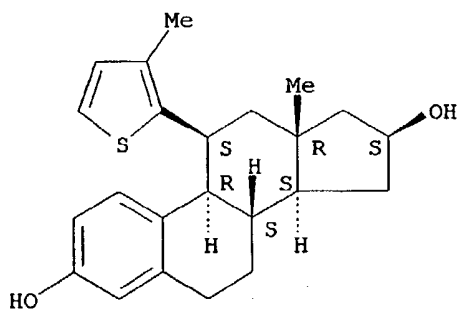
Absolute stereochemistry.



RN 287724-24-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, 11-(3-methyl-2-thienyl)-,
(11.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



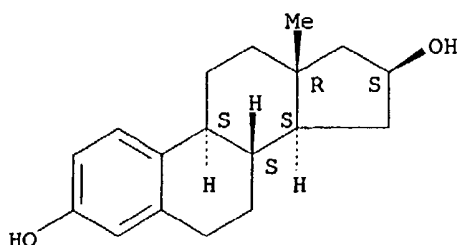
IT 1225-58-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of 16-Hydroxyestratrienes as selectively effective
estrogens)

RN 1225-58-7 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 7 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1999:648063 HCAPLUS
 DOCUMENT NUMBER: 131:332226
 TITLE: Ligand structure influences autologous downregulation of estrogen receptor-alpha messenger RNA
 AUTHOR(S): Davis, M. D.; VanderKuur, J. A.; Brooks, S. C.
 CORPORATE SOURCE: Department of Biochemistry and Molecular Biology and the Barbara Ann Karmanos Cancer Institute, Wayne State University School of Medicine, Detroit, MI, 48201, USA
 SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1999), 70(1-3), 27-37
 CODEN: JSBBEZ; ISSN: 0960-0760
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

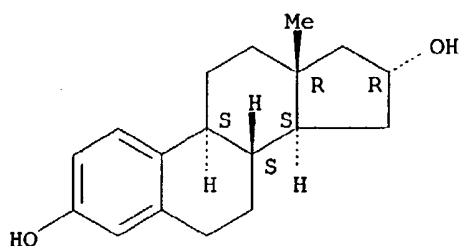
AB A series of A- and D-ring substituted estrogen analogs have been examd. for their effect on estrogen receptor-alpha (ER.alpha.) mRNA downregulation. Recently it has been proposed that ER.alpha. autologous downregulation occurs via transcriptional repression exerted by the binding of the ER.alpha.-ligand complex to the 5' region of the coding region of the ER.alpha. gene. Placement of the phenolic hydroxyl group on the various carbons of the arom. A-ring of estratrien-17.beta.-ol (carbons 1-3) produced ligands which diminished the steady state level of ER.alpha. mRNA in relation to their affinity for receptor. 4-Hydroxyestratrien-17.beta.ol, was inactive in the downregulation of ER.alpha. mRNA. Although this A-ring isomer brought about apparent processing of the nuclear receptor, the ER.alpha. reappeared in the cytosol within 24 h. Unlike the stimulation of genes regulated via estrogen response elements, max. autologous neg. regulation of the ER.alpha. gene required the presence of an hydroxyl group on carbon 17 of the D-ring. These results suggest that the conformational alterations elicited in the ER.alpha. mol. by various ligands create surfaces capable of interacting with other transcription factors in a manner which is different when the receptor functions via a response element mechanism relative to interactions during autologous neg. regulation of the ER.alpha. gene.

IT 1090-04-6
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
 (ligand structure influences autologous downregulation of estrogen receptor-.alpha. mRNA)

RN 1090-04-6 HCAPLUS

CN Estradiol, 17-beta-ol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:424629 HCAPLUS

DOCUMENT NUMBER: 131:223634

TITLE: The two phyto-estrogens genistein and quercetin exert different effects on estrogen receptor function

AUTHOR(S): Miodini, P.; Fioravanti, L.; Di Fronzo, G.; Cappelletti, V.

CORPORATE SOURCE: Istituto Nazionale per lo Studio e la Cura dei Tumori, Milan, Italy

SOURCE: British Journal of Cancer (1999), 80(8), 1150-1155
CODEN: BJCAAI; ISSN: 0007-0920

PUBLISHER: Churchill Livingstone

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors compared the estrogenic and anti-estrogenic properties of the two well-known phyto-estrogens, genistein and quercetin, on the estrogen-sensitive breast cancer cell line MCF-7. Genistein exerted a biphasic effect on growth of MCF-7 cells, stimulating at low and inhibiting at high concns., whereas quercetin was only growth inhibitory. At doses which did not inhibit cell growth, resp. 5 and 1 .mu.M, genistein and quercetin counteracted estrogen- and transforming growth factor-.alpha.-promoted cell growth stimulation. Furthermore, genistein promoted transcription of the estrogen-regulated genes pS2 and cathepsin-D, whereas quercetin interfered with the estrogen-induced expression of the proteins. In in vitro binding expts., genistein competed with estradiol for binding to the estrogen receptor (ER), but quercetin did not. Quercetin and genistein down-regulated cytoplasmic ER levels and promoted a tighter nuclear assocn. of the ER, but only genistein was able to up-regulate progesterone receptor protein levels. In gel mobility assays, ER preincubation with estradiol or with the two phyto-estrogens led to the appearance of the same retarded band, excluding differences between the various complexes in binding to the consensus sequence. The data allowed the authors to conclude that quercetin acts like a pure anti-estrogen, whereas genistein displays mixed agonist/antagonist properties, and to formulate a hypothesis on the possible mechanism of action of such phyto-estrogens.

IT 1090-04-6, 16.alpha.-Estradiol

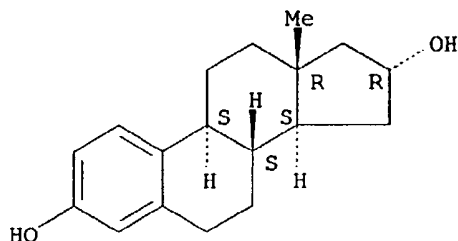
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(quercetin and genistein effect on growth of MCF-7 cell treated with estradiol and growth factors)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:407827 HCAPLUS

DOCUMENT NUMBER: 131:211611

TITLE: Structure and toxicity of the cucurbitacins from *Fevillea cordifolia*AUTHOR(S): Echeverri, Fernando; Torres, Fernando; Lobo, Tatiana
CORPORATE SOURCE: Department of Chemistry, Universidad de Antioquia, Medellin, Colombia

SOURCE: Natural Product Analysis: Chromatography, Spectroscopy, Biological Testing, [Symposium], Wuerzburg, Germany, Sept. 1997 (1998), Meeting Date 1997, 385-386. Editor(s): Schreier, Peter. Vieweg: Wiesbaden, Germany.

CODEN: 67USA7

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Several known fevicordins and two new cucurbitacins whose structures were assigned by 2D NMR were isolated from the seeds of *Fevillea cordifolia*. Although cucurbitacins are just recognized by their toxicity, the compds. isolated from *F. cordifolia* were i.p. inactive in mice at doses of 1.0 and 4.0 mg.

IT 151589-26-3 243139-36-8

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

BIOL (Biological study); OCCU (Occurrence)

(from *Fevillea cordifolia*)

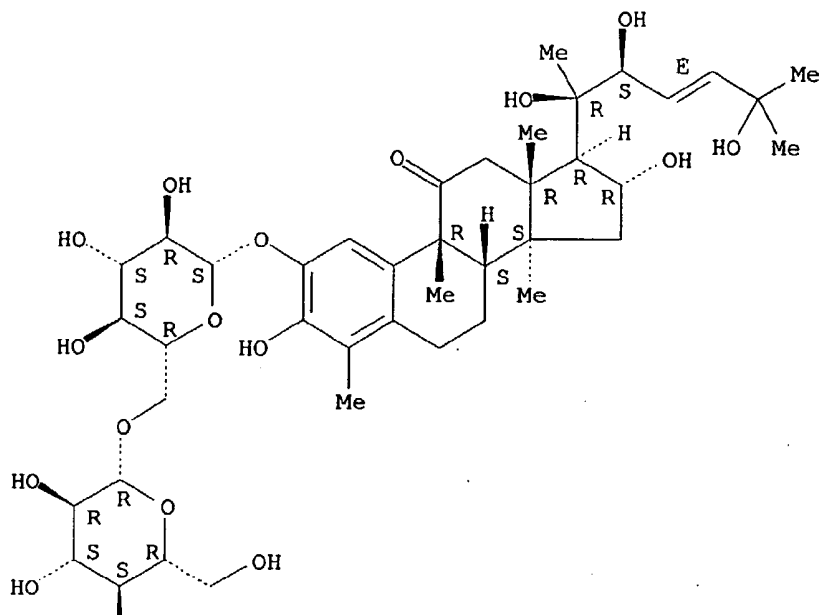
RN 151589-26-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

Double bond geometry as shown.

PAGE 1-A

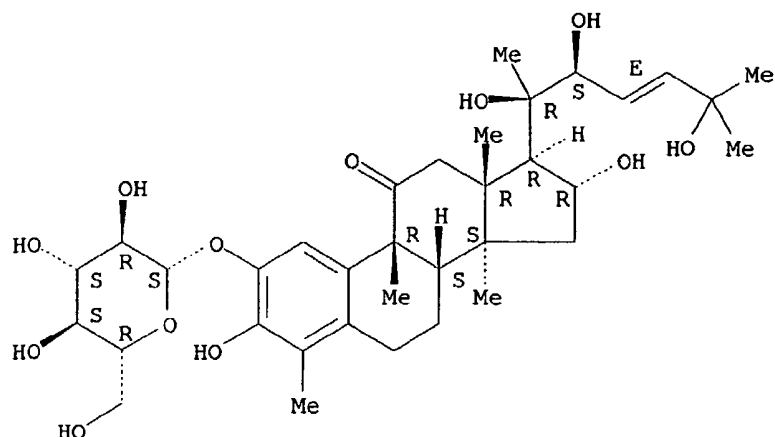


PAGE 2-A



RN 243139-36-8 HCAPLUS
 CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-
 3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,22S,23E)-
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



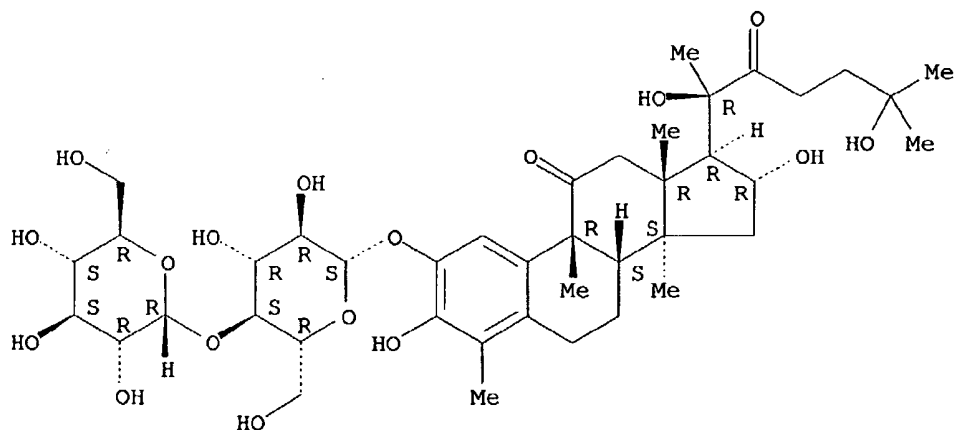
IT 243116-46-3P 243116-47-4P

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(from *Fevillea cordifolia*)

RN 243116-46-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-[(4-O-.alpha.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,25-tetrahydroxy-4,9,14-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

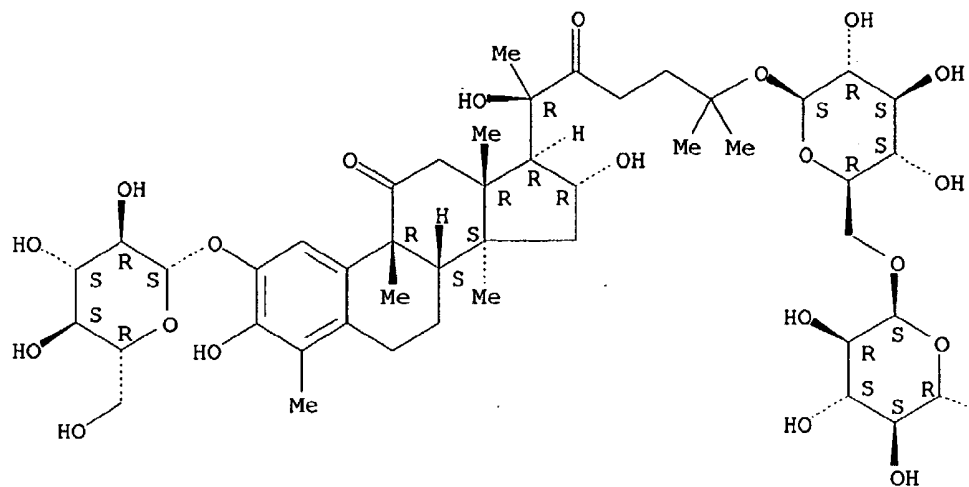


RN 243116-47-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-[(6-O-.alpha.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



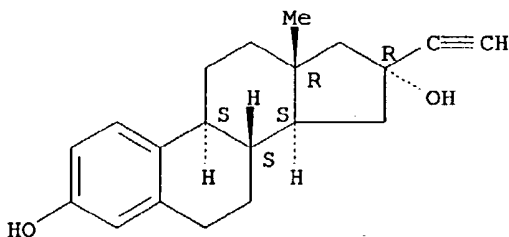
PAGE 1-B



L5 ANSWER 10 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1998:559789 HCAPLUS
 DOCUMENT NUMBER: 129:306174
 TITLE: Analysis of potential endocrine disrupting chemicals
 in sewage effluents using continuous liquid-liquid
 extraction with derivatization and gas
 chromatography/mass spectrometry analysis
 AUTHOR(S): Barber, Larry B.; Brown, Greg K.; Writer, Jeffery H.;
 Zaugg, S. A.
 CORPORATE SOURCE: U. S. Geological Survey, Boulder, CO, 80303, USA
 SOURCE: Preprints of Extended Abstracts presented at the ACS
 National Meeting, American Chemical Society, Division
 of Environmental Chemistry (1998), 38(2), 273-275

CODEN: PEACF2
 PUBLISHER: American Chemical Society, Division of Environmental Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Anal. of potential endocrine disrupting chems. in wastewater effluent using continuous liq.-liq. extn. with derivatization and gas chromatog./mass spectrometry anal. is described.
 IT 24989-47-7
 RL: ANT (Analyte); ANST (Analytical study)
 (endocrine disrupting chems. detn. in wastewater by continuous liq.-liq. extn. with derivatization and gas chromatog./mass spectrometry anal. under base, neutral, and acid conditions)
 RN 24989-47-7 HCAPLUS
 CN Estradiol-1,3,5(10)-triene-3,16-diol, 16-ethynyl-, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1997:638466 HCAPLUS
 DOCUMENT NUMBER: 127:288310
 TITLE: Induction of the Estrogen Specific Mitogenic Response of MCF-7 Cells by Selected Analogs of Estradiol-17.beta.: A 3D QSAR Study
 AUTHOR(S): Wiese, Thomas E.; Polin, Lisa A.; Palomino, Eduardo; Brooks, S. C.
 CORPORATE SOURCE: Department of Biochemistry, Wayne State University
 School of Medicine, Detroit, MI, 48201, USA
 SOURCE: Journal of Medicinal Chemistry (1997), 40(22), 3659-3669
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Analogs of estradiol-17.beta. (E2) have been evaluated for estrogen receptor (ER) binding affinity and mitogenic potential in the human breast cancer cell line MCF-7. These 42 compds. represent subtle modifications of the natural estrogen structure through the placement of hydroxyl, amino, nitro, or iodo groups around the ring system in addn. to, or as replacement of, the 3- and 17.beta.-hydroxyls of E2. The mitogenic activity of the analogs was found to be related to ER binding only to a limited extent. To elucidate structural features that are uniquely responsible for receptor binding affinity or mitogen potential of estrogens, the three-dimensional quant. structure-activity (QSAR) method

Comparative Mol. Field Anal. (CoMFA) was employed. Sep. CoMFA models for receptor binding and cell growth stimulation were optimized through the use of various alignment rules and region step size. Whereas the CoMFA contour plots did outline the shared structural requirements for the two measured biol. properties, specific topol. features in this set of estrogens were delineated that distinguish mitogenic potential from ER binding ability. In particular, steric interference zones which affected growth extend in a band from above the A-ring to position 4 and below, whereas the ER binding steric interference zones are limited to isolated polyhedra in the 1,2 and 4 positions and the .alpha. face of the B-ring. In addn., electroneg. features located around the A-, B-, or C-rings contribute to receptor affinity. However, growth is dependent only on electroneg. and electropos. properties near the 3-position. In a final QSAR model for the mitogenic response, the value of ER binding was included along with structural features as a descriptor in CoMFA. The resulting 3D-QSAR has the most predictive potential of the models in this study and can be considered a prototype model for the general evaluation of a steroidal estrogen's growth stimulating ability in MCF-7 cells. For example, the location of D-ring contours illustrate the model's preference for 17.beta.-hydroxy steroids over the less mitogenic 17.alpha.- and 16.alpha.-hydroxy compds. In addn., the enhanced mitogenic effect of steric bulk in the 11.alpha.-position is also evident. The QSAR studies in this report illustrate the fact that while ER binding may be a required factor of the estrogen dependent growth response in MCF-7 cells, particular structural characteristics, in addn. to those responsible for tight receptor binding, must be present to induce an optimal mitogenic response. Therefore, this report demonstrates that the CoMFA QSAR method can be utilized to characterize structural features of test compds. that account for different types of estrogenic responses.

IT 1090-04-6

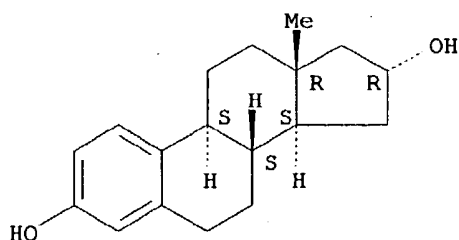
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(3D QSAR study of induction of estrogen specific mitogenic response of MCF-7 cells by selected analogs of estradiol)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 12 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:244398 HCAPLUS

DOCUMENT NUMBER: 126:225448

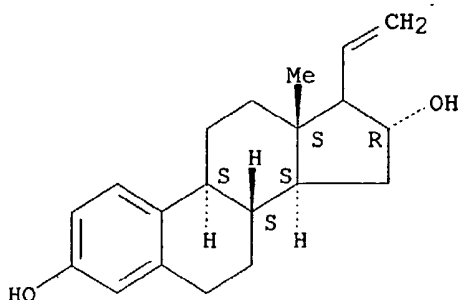
TITLE: Novel estrogens for treating autoimmune diseases

INVENTOR(S): Brattsand, Ralph; Holmdahl, Rikard; Jansson, Liselotte; Loncar, Marjana; Pettersson, Lars

PATENT ASSIGNEE(S): Astra Aktiebolag, Swed.; Brattsand, Ralph; Holmdahl, Rikard; Jansson, Liselotte; Loncar, Marjana; Pettersson, Lars
 SOURCE: PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9708188	A1	19970306	WO 1996-SE1028	19960820
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
CA 2228803	AA	19970306	CA 1996-2228803	19960820
AU 9668405	A1	19970319	AU 1996-68405	19960820
EP 847399	A1	19980617	EP 1996-928771	19960820
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
JP 11511457	T2	19991005	JP 1997-510174	19960820
US 6043236	A	20000328	US 1997-817683	19970423
PRIORITY APPLN. INFO.: SE 1995-2921 A 19950823 WO 1996-SE1028 W 19960820				
OTHER SOURCE(S): MARPAT 126:225448				
AB Estratrienes I [R = H, alkyl, cycloalkyl, acyl, alkoxycarbonyl, aralkoxycarbonyl, protective group; R1, R2 = H, Me, Et, halogen; R3 = H, acyl, alkoxycarbonyl, aralkoxycarbonyl; R4 = H, Me, Et; Y = CH2, bond] were prepd. Thus, estrone was converted to its 3-dimethylthexyl ether which was treated with EtPPh3+ Br-, followed by SeO2-Me3COOH oxidn. and desilylation to give (17E)-3,16.alpha.-dihydroxy-19-norpregna-1,3,5(10),17(20)-tetraene. I show very low sex hormone side effects while retaining their antiinflammatory and immunosuppressant activity.				
IT 188291-28-3P RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of estratriene derivs. as inflammation inhibitors and immunosuppressants)				
RN 188291-28-3 HCAPLUS				
CN 19-Norpregna-1,3,5(10),20-tetraene-3,16-diol, (16.alpha.,17.xi.)- (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



L5 ANSWER 13 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:683463 HCAPLUS

DOCUMENT NUMBER: 126:57556

TITLE: Geodisterol, a novel polyoxygenated sterol with an aromatic A ring from the tropical marine sponge *Geodia* sp.

AUTHOR(S): Wang, Gui-Yang-Sheng; Crews, Phil

CORPORATE SOURCE: Dep. Chem. and Biochem., Univ. of California, Santa Cruz, CA, 95064, USA

SOURCE: Tetrahedron Letters (1996), 37(45), 8145-8146

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Geodisterol (I), the first marine polyoxygenated sterol with an arom. A ring, was isolated from the Indo-Pacific sponge *Geodia* sp. The structural and stereochem. features of I were based on the extensive anal. of 1D and 2D of it and MPA esters.

IT **185146-75-2P**

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

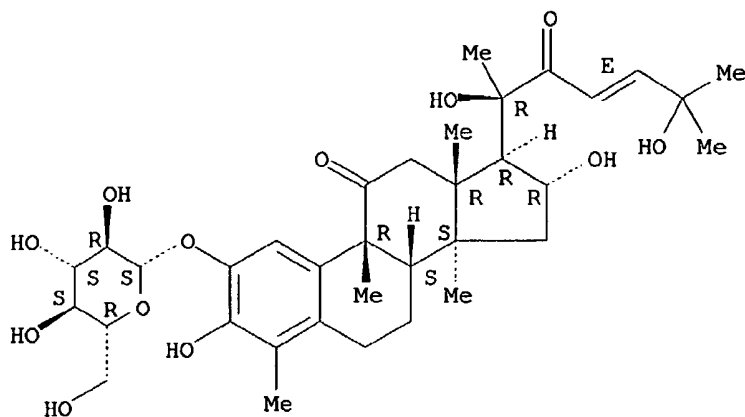
(geodisterol isolation and structural characterization from tropical marine sponge)

RN 185146-75-2 HCAPLUS

CN 19-Norstigmasta-1,3,5(10),24(28)-tetraene-3,16,20-triol, (16.beta.,24E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



L5 ANSWER 17 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:651424 HCAPLUS

DOCUMENT NUMBER: 123:48115

TITLE: Cellular localization of estradiol-induced c-fos messenger ribonucleic acid in the rat uterus: c-fos expression and uterine cell proliferation do not correlate strictly

AUTHOR(S): Nephew, Kenneth P.; Peters, Gregory A.; Khan, Sohaib A.

CORPORATE SOURCE: Coll. Med., Univ. Cincinnati, Cincinnati, OH, 45267-0521, USA

SOURCE: Endocrinology (1995), 136(7), 3007-15

CODEN: ENDOAO; ISSN: 0013-7227

PUBLISHER: Endocrine Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Estrogens stimulate DNA synthesis and cell proliferation in the uterus. All major uterine cell types (luminal and glandular epithelium, stroma, and myometrium) respond to 17.β-estradiol in the immature animal, whereas primarily epithelial cells of the uterine endometrium respond in the mature animal. Rapid activation of the c-fos protooncogene by estrogen precedes the uterine growth, suggesting that c-fos plays a role in amplifying the hormonal signal. The specific uterine cell types in which estrogen induces c-fos mRNA expression, however, have not been identified in either mature or immature animals. In this study, in situ hybridization was used to determine the cell type-specific location of mRNA encoding c-fos in the uterus. In both immature and mature castrated rats at 3 h after 17.β-estradiol administration, c-fos expression was detected primarily in uterine luminal and glandular epithelia. Expression of c-fos returned to baseline levels by 24 h post 17.β-estradiol treatment. There was no apparent difference in the uterine cell type-specific pattern of c-fos expression stimulated by estradiol in mature vs. immature animals. Nuclear run-on transcription assay in isolated luminal epithelial cell nuclei showed that c-fos gene transcription increased rapidly in the uterus after estradiol stimulation. Treatment of adult rats with a single injection of 16.α-estradiol, a short-acting, nonmitogenic estrogen, induced c-fos primarily in the uterine glandular epithelia. Progesterone is known to modify the action of estrogen on the uterus by redirecting the proliferative response from

epithelia to stroma. To det. if progesterone modulation of estrogen action involves shifting of c-fos expression to stromal cells, rats were treated with progesterone for 48 h and then killed 0, 3, 6, or 12 h after an estradiol injection. In situ hybridization anal. revealed that c-fos mRNA remained localized in the uterine luminal and a glandular epithelia, and expression was not shifted to the stroma. Although these results support the idea that c-fos plays a role in proliferation of uterine epithelial cells, they also invite reassessment of the role played by c-fos in both epithelial and nonepithelial uterine cell types.

IT 1090-04-6, 16.alpha.-Estradiol

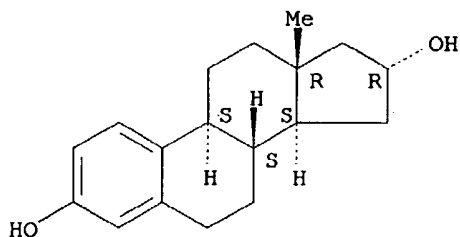
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(cellular localization of estradiol-induced c-fos mRNA in uterus in relation to cell proliferation)

RN 1090-04-6 HCAPLUS

CN Estr-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 18 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:585753 HCAPLUS

DOCUMENT NUMBER: 122:306705

TITLE: Induction of tissue plasminogen activator mRNA and activity by structurally altered estrogens

AUTHOR(S): Davis, M. D.; Butler, W. B.; Brooks, S. C.

CORPORATE SOURCE: Dep. Biochemistry, Wayne State Univ. School Medicine, USA

SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1995), 52(5), 421-30

CODEN: JSBBEZ; ISSN: 0960-0760

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of structure of the estrogen ligand on the accumulation of tPA mRNA and the activity of extracellular fibrinolytic enzyme has been examd. in cultures of MCF-7 cells. Estradiol (E2)-stimulated fibrinolytic activity was preceded by an increase in actinomycin D sensitive tPA mRNA synthesis which peaked at 18 h. Ten A- and D-ring structural analogs of E2 affected tPA mRNA accumulation and extracellular fibrinolytic activity. Only in the case of two A-ring isomers (2- and 4-hydroxyestratrien-17.beta.-ol) was the decreased effect of the ligand's structural change on tPA mRNA accumulation and fibrinolysis not explained by a comparable decline in affinity of the ligand for estrogen receptor. Both of these analogs functioned as antiestrogens. The stimulatory capacity of

androstane diols on the tPA gene required that the 3-hydroxyl group be positioned in the .beta.-configuration. Absence of the 17.beta.-hydroxy group was beneficial to the max. accumulation of tPA mRNA. As has been reported for other estrogen responsive genes (progesterone receptor, cathepsin D and pS2), regulation by estrogens is not related directly to the affinity of the ligand for ER, but this activity may be detd. by the location of the electroneg. isopotential above the A-ring of estrogenic ligands.

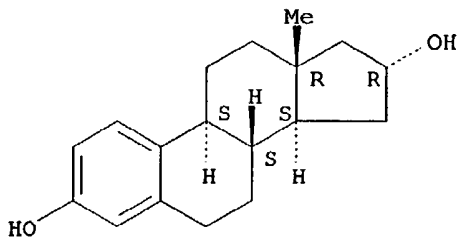
IT 1090-04-6, 16.alpha.-Estradiol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(tissue plasminogen activator induction by structurally altered estrogens)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 19 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:441845 HCAPLUS

DOCUMENT NUMBER: 122:281523

TITLE: Inhibitory effects of cucurbitane triterpenoids on Epstein-Barr virus activation and two-stage carcinogenesis of skin tumor. II

AUTHOR(S): Konoshima, Takao; Takasaki, Midori; Kozuka, Mutsuo; Nagao, Tsuneatsu; Okabe, Hikaru; Irino, Nobuto; Nakasumi, Tetsuo; Tokuda, Harukuni; Nishino, Hoyoku
CORPORATE SOURCE: Kyoto Pharm. Univ., Kyoto, 607, Japan

SOURCE: Biological & Pharmaceutical Bulletin (1995), 18(2), 284-7

CODEN: BPBLEO; ISSN: 0918-6158

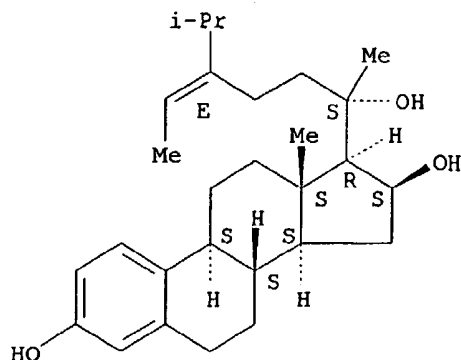
PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To search for possible anti-tumor-promoters, we carried out a primary screening of twenty-four 29-nor-cucurbitacin glucosides isolated from the roots of Cayaponia tayuya (Cucurbitaceae) using an in vitro synergistic assay system. Of these glucosides, cayaponosides B (5), B3 (7), D (8), D3b (22) and C2 (23) exhibited significant inhibitory effects on Epstein-Barr virus (EBV) activation induced by the tumor promoter, 12-O-tetradecanoylphorbol-13-acetate (TPA). Furthermore, 5 and 23 exhibited remarkable anti-tumor-promoting effects on mouse skin tumor promotion in an in vivo two-stage carcinogenesis test.

IT 147742-04-9, Cayaponoside A 147742-05-0, Cayaponoside B
147742-06-1, Cayaponoside C 147764-94-1, Cayaponoside D



L5 ANSWER 14 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1996:449391 HCAPLUS
 DOCUMENT NUMBER: 125:81803
 TITLE: Studies on the Constituents of *Cyclanthera pedata* (Caigua) Seeds: Isolation and Characterization of Six New Cucurbitacin Glycosides
 AUTHOR(S): De Tommasi, Nunziatina; De Simone, Francesco; Pizza, Cosimo
 CORPORATE SOURCE: Facolta di Farmacia, Universita di Salerno, Penta di Fisciano, 84084, Italy
 SOURCE: Journal of Agricultural and Food Chemistry (1996), 44(8), 2020-2025
 CODEN: JAFCAU; ISSN: 0021-8561
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Six new cucurbitacin glycosides were isolated from the seeds of *Cyclanthera pedata* Schrab (Cucurbitaceae). Their structures were elucidated on the basis of spectral and chem. data to be 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16.alpha.,20,22,25-pentahydroxy-29-norcucurbita-1,3,5(10)-trien-11-one, 25-acetoxy-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16.alpha.,20,22-tetrahydroxy-29-norcucurbita-1,3,5(10)-trien-11-one, 25-acetoxy-2-(.beta.-D-glucopyranosyloxy)-3,16.alpha.,20,22-tetrahydroxy-29-norcucurbita-1,3,5(10)-trien-11-one, 25-acetoxy-2-[(4-O-.alpha.-L-rhamnopyranosyl-6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16.alpha.,20-trihydroxy-29-norcucurbita-1,3,5(10)-triene-11,22-dione, 3.beta.-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-16.alpha.,20,22,25-tetrahydroxycucurbit-5-en-11-one, and 3-.beta.-(.beta.-D-glucopyranosyloxy)-25-acetoxy-16.alpha.,20,22,-trihydroxycucurbit-5-en-11-one.

IT 178062-90-3P 178062-91-4P 178062-92-5P
 178062-93-6P

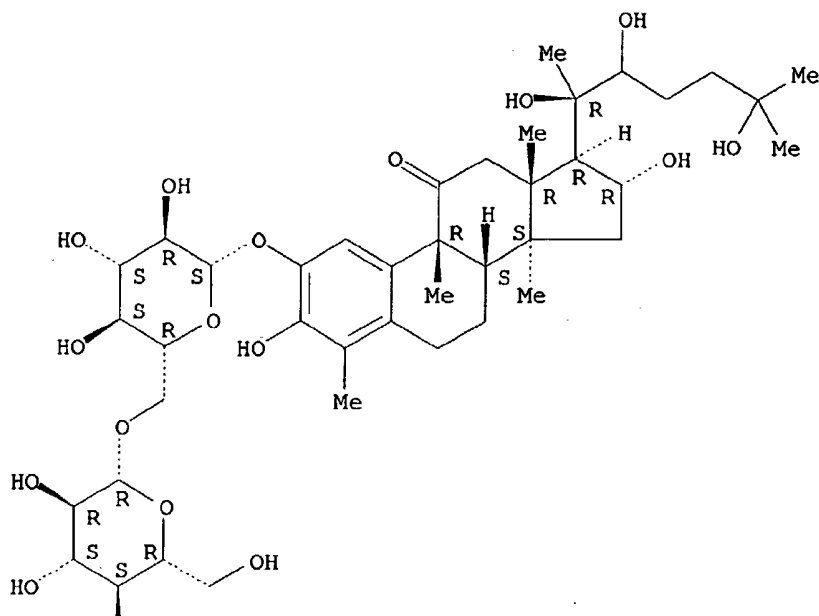
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (isolation from *Cyclanthera pedata* seeds and structure of)

RN 178062-90-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22-tetrahydroxy-25-hydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A

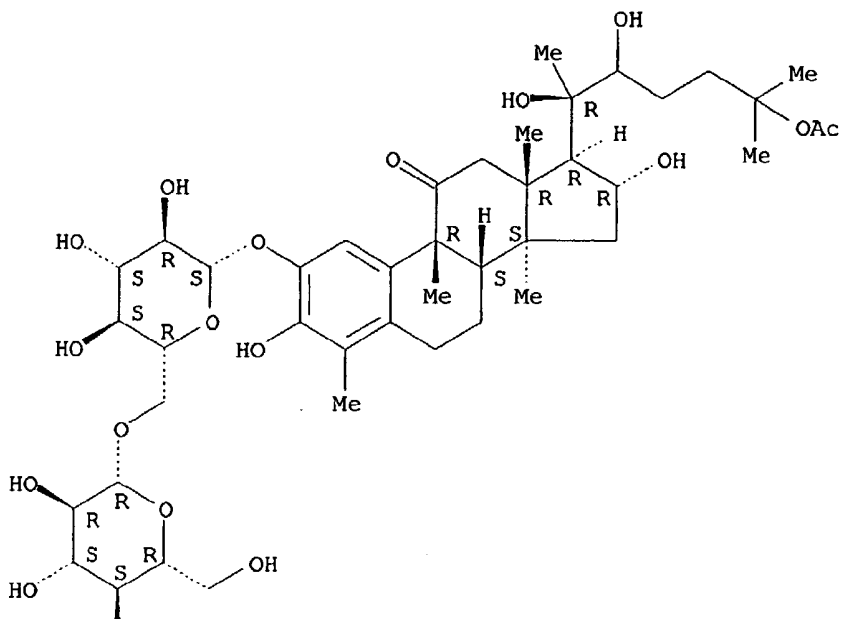


RN 178062-91-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 25-(acetyloxy)-2-[(6-O-.beta.-D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



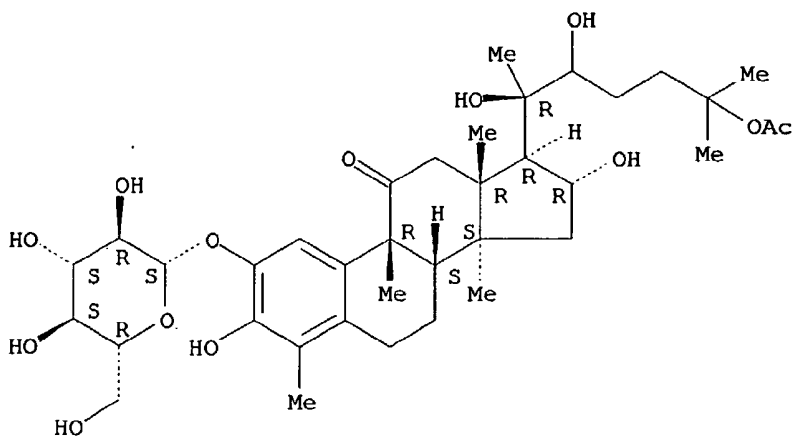
PAGE 2-A

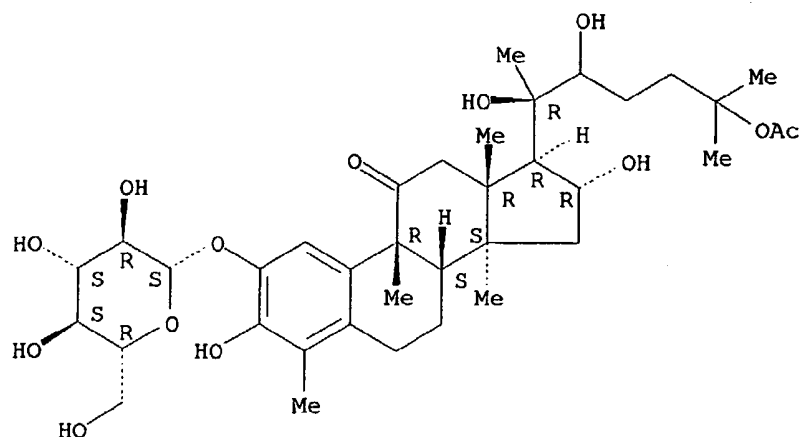


RN 178062-92-5 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



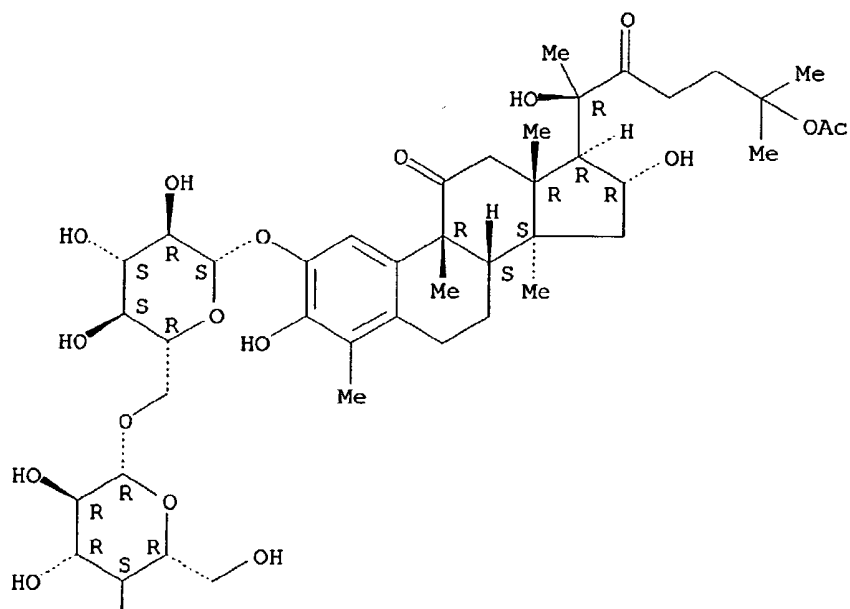


RN 178062-93-6 HCAPLUS

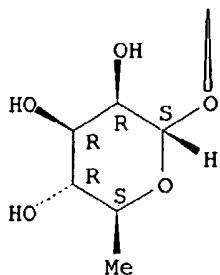
CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-[(O-6-deoxy-.alpha.-L-mannopyranosyl-(1.fwdarw.4)-O-.beta.-D-glucopyranosyl-(1.fwdarw.6)-.beta.-D-glucopyranosyl)oxy]-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



PAGE 2-A



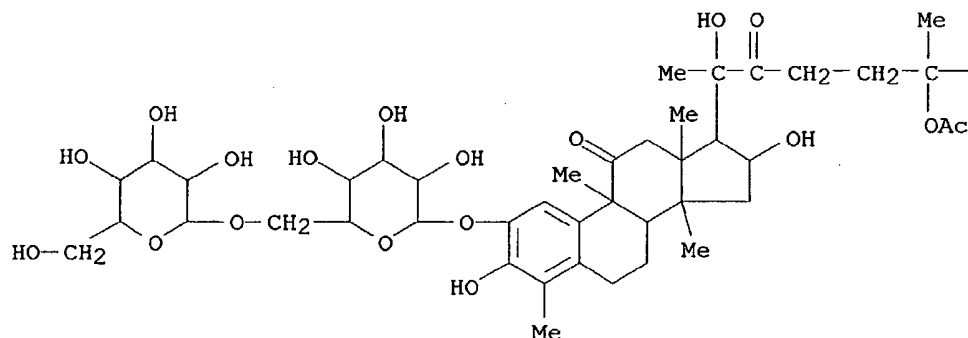
IT 151589-22-9

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);
 BIOL (Biological study); OCCU (Occurrence)
 (of *Cyclanthera pedata* seeds)

RN 151589-22-9 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-[(6-O-.beta.-
 D-glucopyranosyl-.beta.-D-glucopyranosyl)oxy]-3,16,20-trihydroxy-4,9,14-
 trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— Me

L5 ANSWER 15 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:901632 HCAPLUS

DOCUMENT NUMBER: 123:306774

TITLE: Relationship between estrogen structure and
 conformational changes in estrogen receptor/DNA
 complexes

AUTHOR(S): Christman, J. K.; Nehls, S.; Polin, L.; Brooks, S. C.

CORPORATE SOURCE: Molecular Biology Program, Michigan Cancer Foundation,
 Detroit, MI, 48201, USA

SOURCE: Journal of Steroid Biochemistry and Molecular Biology

(1995), 54(5/6), 201-10
CODEN: JSBBEZ; ISSN: 0960-0760

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

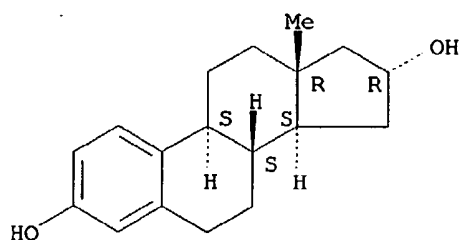
AB The effect of estrogen structure on the conformation of the complex formed with estrogen receptor (ER) and the consensus estrogen response element (EREc) has been examd. with gel mobility shift assay. Proteins in MCF-7 cell exts. formed three distinct complexes with ERE. Only the slowest moving complex contained ER as indicated by binding with anti-ER antibodies H222 and D547. This ER-ERE complex displayed increased electrophoretic mobility when formed in the presence of estradiol (E2) and bound radiolabeled 16.alpha.-iodoestradiol. The antiestrogen ICI 164384 decreased the mobility of the ER-ERE complex and blocked the effect of E2. The results reported here indicate that the position and location of hydroxyl groups on the estratriene nucleus is an important factor in detg. the mobility of ER-EREc (or a variant ERE) in gel shift assays. The ability of E2 analogs to cause conformational changes detectable as altered mobility was not directly related either to their binding affinity for ER or to their ability to activate E2 responsive genes. Although several dihydroxy estrogens (estradiol-16.alpha., 1- and 2-hydroxyestratrien-17.beta.-ol) caused an increased in the mobility of the ER-EREc, other ligands (estradiol-17.alpha., 4-hydroxyestratrien-17.beta.-ol, 3-hydroxyestratriene, estratrien-17.beta.-ol and 5-androstene-3.beta.,17.beta.-diol) with a capacity for activating at least some E2 responsive genes in MCF-7 cells had little or no effect. On the basis of these and previously published results, it can be concluded that specific structures of estrogens are responsible for conformational changes of ER-ERE complexes detectable in gel-shift assays. Furthermore, the identified structural characteristics of the ligand which are required for gel-shift are not the same as those previously reported to be essential for stimulation of transcriptional activity of ER.

IT 1090-04-6, 16.alpha.-Estradiol
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(estrogen structure in relation to conformational changes in estrogen receptor-estrogen-responsive element complexes)

RN 1090-04-6 HCAPLUS

CN Estra-1,3,5(10)-triene-3,16-diol, (16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 16 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:766521 HCAPLUS
DOCUMENT NUMBER: 123:222777

TITLE: Constituents of tropical medicinal plants. LXVII:
24-Acetylaminofevicordin D glucoside, an artificial
constituent of *Fevillea cordifolia*? On the reactivity
of fevicordins

AUTHOR(S): Achenbach, Hans; Horn, Konrad; Waibel, Reiner

CORPORATE SOURCE: Institut Pharmazie lebensmittelchemie, Universitaet
Erlangen, Erlangen, 91052, Germany

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1995),
328(6), 481-5
CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER: VCH

DOCUMENT TYPE: Journal

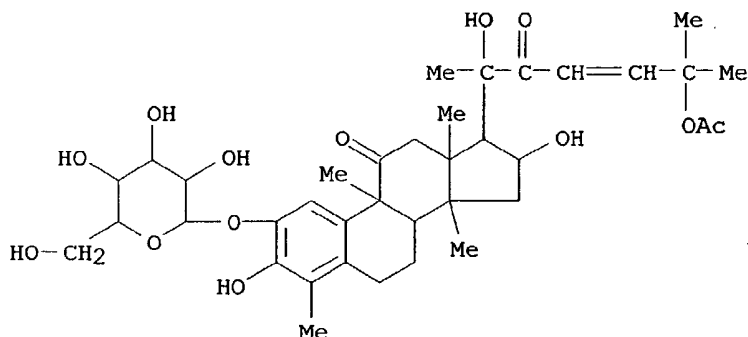
LANGUAGE: German

AB 24-Acetylaminofevicordin D glucoside (I) was isolated as a minor component from the seeds of *Fevillea cordifolia* (Cucurbitaceae) and its structure was detd. by spectroscopic methods. Expts. showed that the enone-system in the side chain of fevicordin A glucoside, which represents the main constituent of the seeds, undergoes a Michael addn. with nucleophiles, and ammonia reacts very easily under simultaneous migration of the acetyl group from C-25 to the nitrogen. Therefore, I probably has to be regarded as an artifact.

IT **111250-01-2**, Fevicordin A glucoside
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(Michael addn. and NMR data and reactivity of)

RN 111250-01-2 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

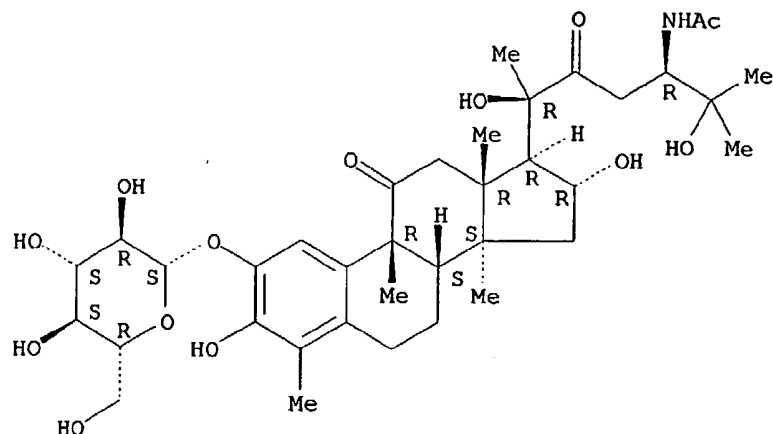


IT **168287-72-7P 168287-76-1P**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)
(isolation as artifact from *Fevillea* and NMR data and prepn. and acetylation of)

RN 168287-72-7 HCAPLUS

CN Acetamide, N-[(9.beta.,16.alpha.,24R)-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-11,22-dioxo-19-norcholesta-1,3,5(10)-trien-24-yl]- (9CI) (CA INDEX NAME)

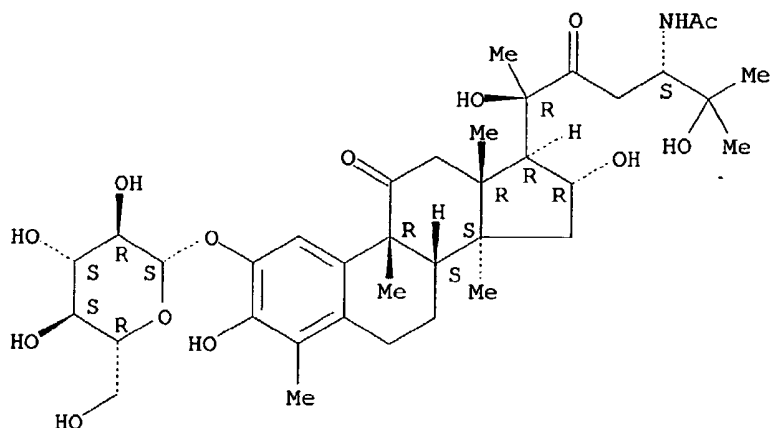
Absolute stereochemistry. Rotation (-).



RN 168287-76-1 HCAPLUS

CN Acetamide, N-[(9.beta.,16.alpha.,24S)-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-11,22-dioxo-19-norcholesta-1,3,5(10)-trien-24-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



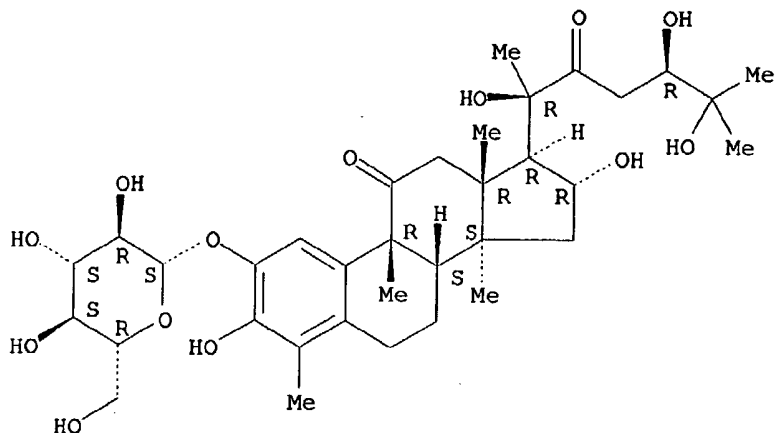
IT 168287-73-8P 168287-77-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and NMR data of)

RN 168287-73-8 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,24,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24R)- (9CI) (CA INDEX NAME)

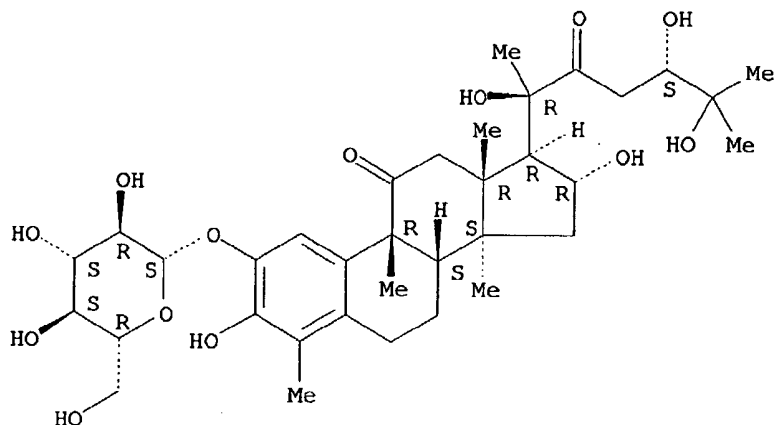
Absolute stereochemistry.



RN 168287-77-2 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,24,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



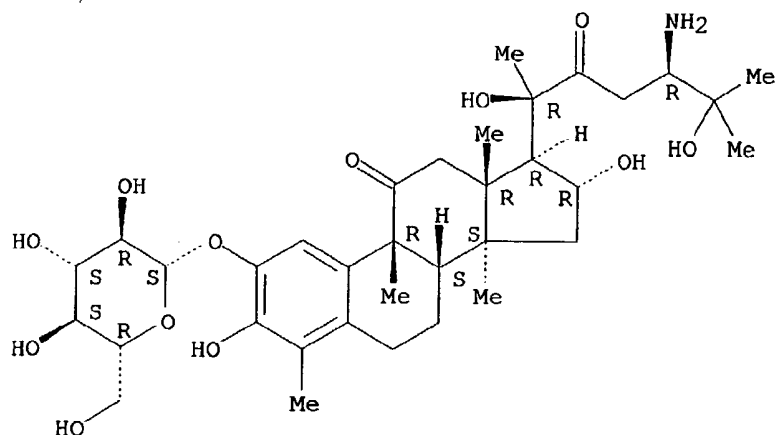
IT 168287-74-9P 168287-78-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and acetylation and NMR data of)

RN 168287-74-9 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 24-amino-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24R)- (9CI) (CA INDEX NAME)

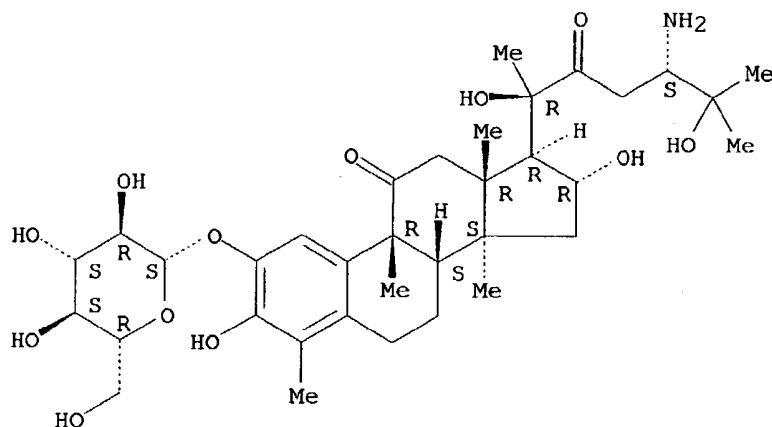
Absolute stereochemistry.



RN 168287-78-3 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 24-amino-2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,24S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 151589-19-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reactions with ammonia and KOH)

RN 151589-19-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

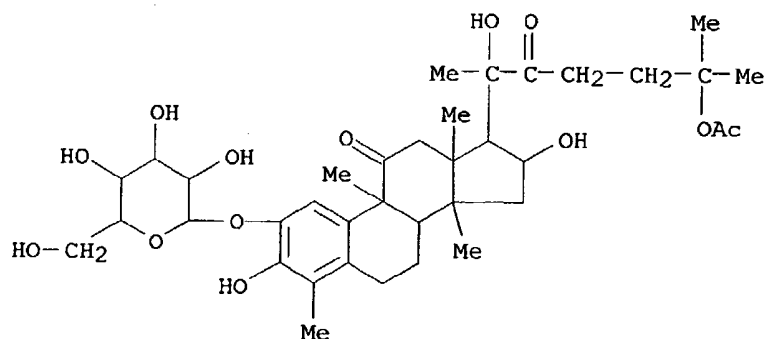
151589-19-4, Cayaponoside C5a 151703-09-2, Cayaponoside B4 151703-10-5, Cayaponoside C2 162857-56-9, Cayaponoside A3 162857-57-0, Cayaponoside A4 162857-58-1, Cayaponoside A6 162857-59-2, Cayaponoside B2 162857-60-5, Cayaponoside B3 162857-61-6, Cayaponoside D1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(cucurbitane triterpenoids inhibition of Epstein-Barr virus and two-stage carcinogenesis of skin tumor)

RN 147742-04-9 HCAPLUS

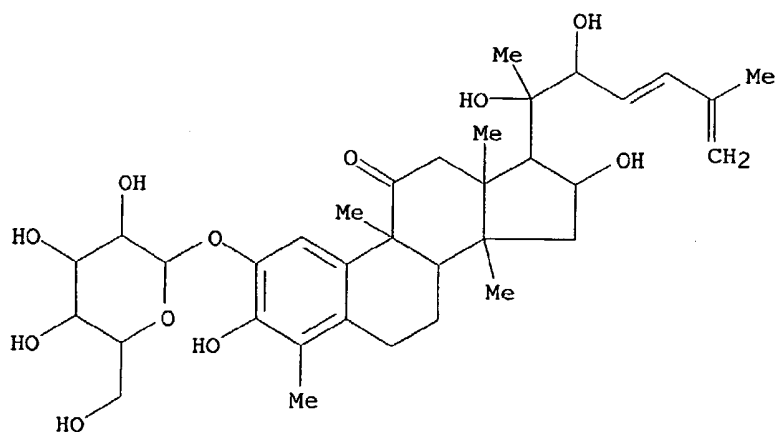
CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 147742-05-0 HCAPLUS

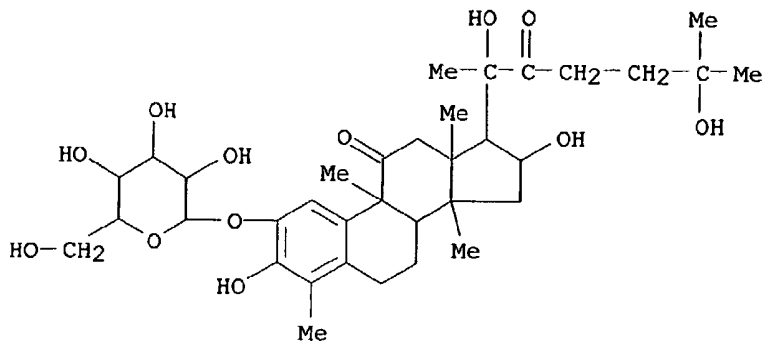
CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 147742-06-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



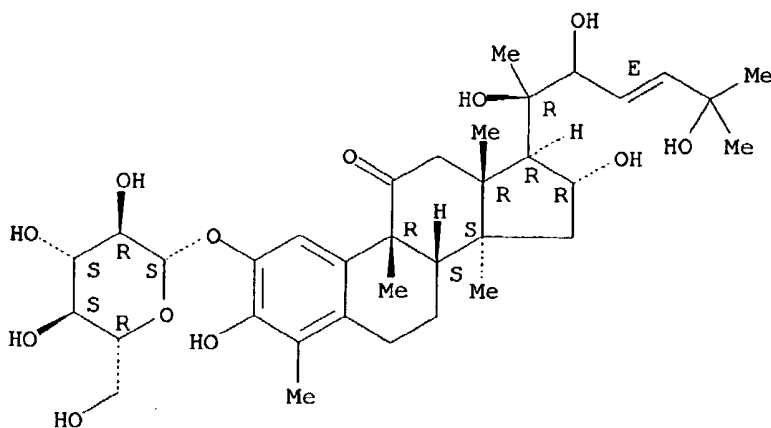
RN 147764-94-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Currently available stereo shown.

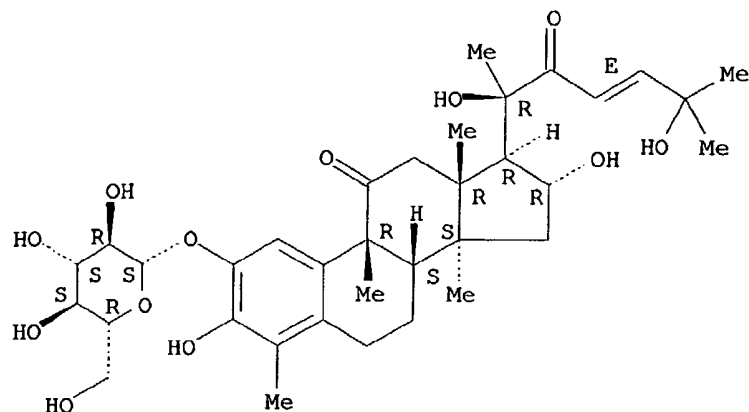


RN 151589-19-4 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

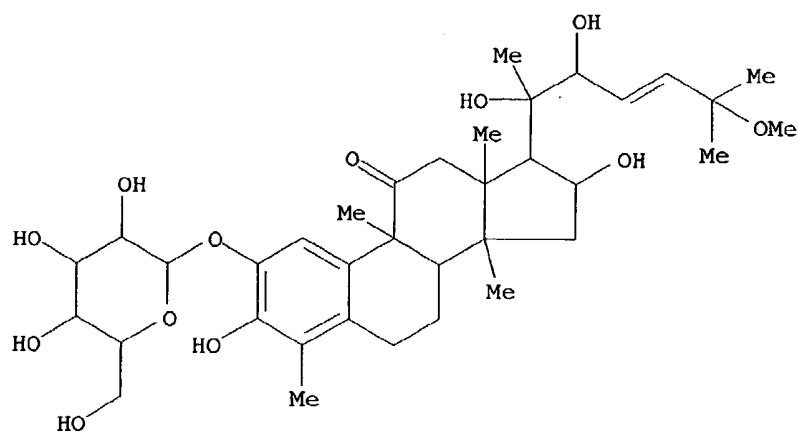
Double bond geometry as shown.



RN 151703-09-2 HCAPLUS

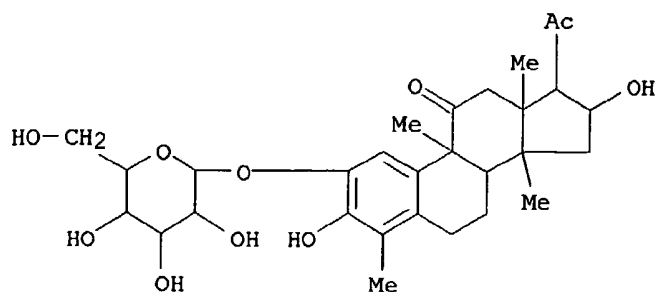
CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-25-methoxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)-(9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 151703-10-5 HCAPLUS

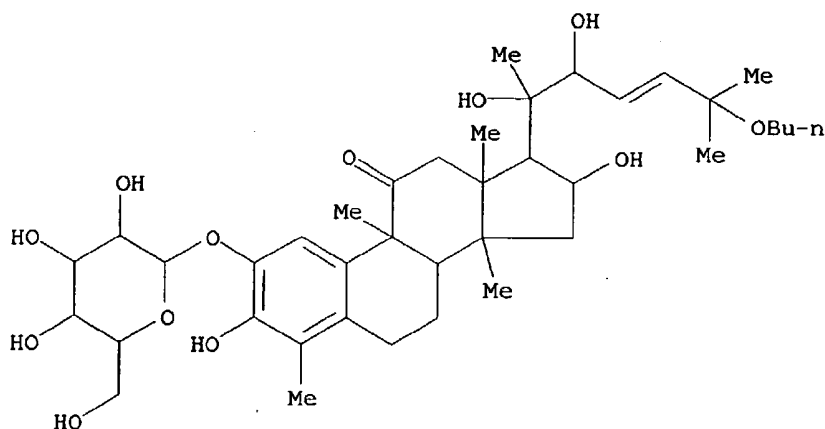
CN 19-Norpregna-1,3,5(10)-triene-11,20-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16-dihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)-(9CI) (CA INDEX NAME)



RN 162857-56-9 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23-tetraen-11-one, 25-butoxy-2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.,23E)- (9CI) (CA INDEX NAME)

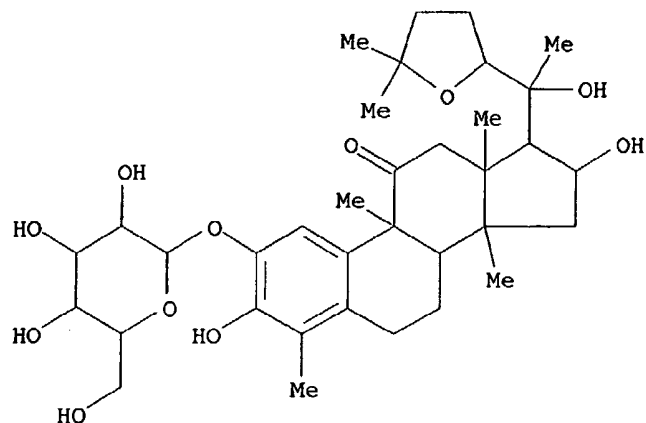
Currently available stereo shown.



RN 162857-57-0 HCAPLUS

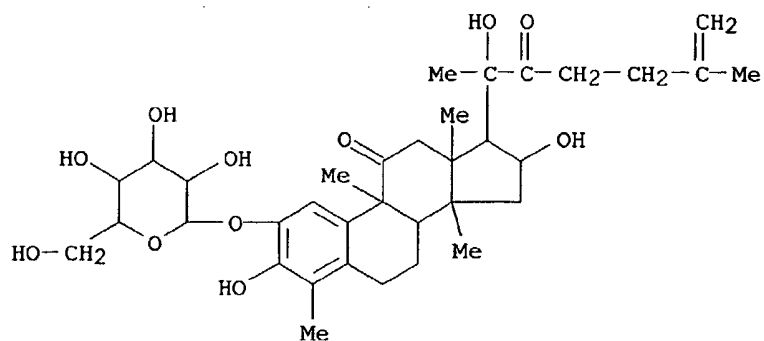
CN 19-Norcholesta-1,3,5(10)-trien-11-one, 22,25-epoxy-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 162857-58-1 HCAPLUS

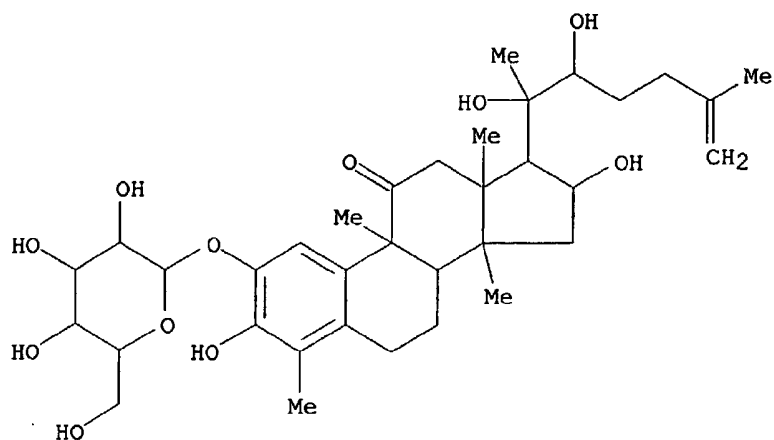
CN 19-Norcholesta-1,3,5(10),25-tetraene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 162857-59-2 HCAPLUS

CN 19-Norcholesta-1,3,5(10),25-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

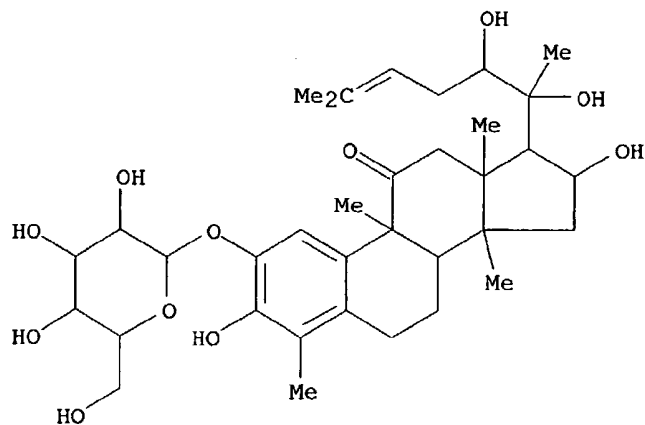
Currently available stereo shown.



RN 162857-60-5 HCAPLUS

CN 19-Norcholesta-1,3,5(10),24-tetraen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

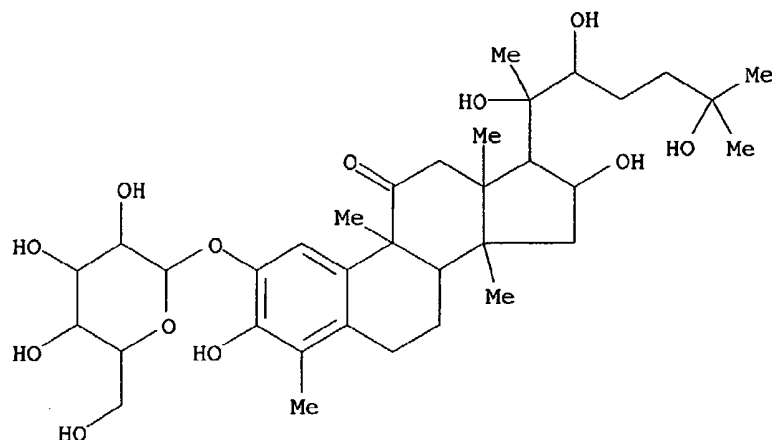
Currently available stereo shown.



RN 162857-61-6 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-trien-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22,25-pentahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



L5 ANSWER 20 OF 90 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:441021 HCAPLUS

DOCUMENT NUMBER: 122:286614

TITLE: Studies on the constituents of the root of *Cayaponia tayuya* (Vell.) Cogn. I. Structures of cayaponosides, new 29-nor-1,2,3,4,5,10-hexadehydrocucurbitacin glucosides

AUTHOR(S): Himeno, Eiji; Nagao, Tsuneatsu; Honda, Junko; Okabe, Hikaru; Irino, Nobuto; Nakasumi, Tetsuo

CORPORATE SOURCE: Fac. Pharm. Sci., Fukuoka Univ., Fukuoka, 814-01, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(11), 2295-300

CODEN: CPBTAL; ISSN: 0009-2363

PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The bitter constituents in the root of *Cayaponia tayuya* (Vell.) Cogn. were investigated, and 24 29-norcucurbitacin glucosides, named cayaponosides, were isolated. Among them, the structures of cayaponosides A, A3, A4, A6, B, B2, B3, B4, C, C2, C5a, D and D1 were detd. based mainly on spectral analyses. They are all glucosides of 29-nor-1,2,3,4,5,10-hexadehydrocucurbitacins, different only in side chain structure.

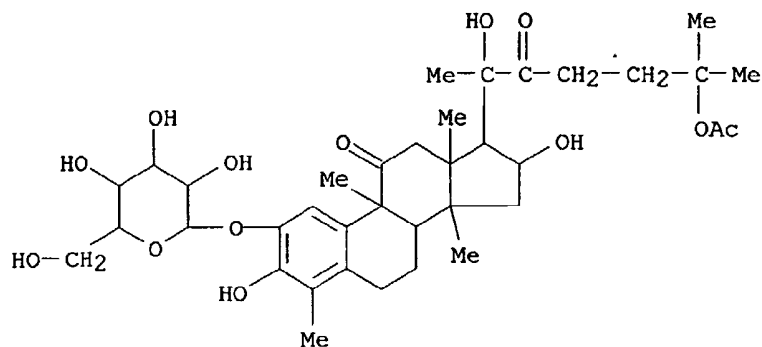
IT 147742-04-9P, Cayaponoside A 147742-05-0P, Cayaponoside B 147742-06-1P, Cayaponoside C 147764-94-1P, Cayaponoside D 151589-19-4P, Cayaponoside C5a 151703-09-2P, Cayaponoside B4 151703-10-5P, Cayaponoside C2 162857-56-9P, Cayaponoside A3 162857-57-0P, Cayaponoside A4 162857-58-1P, Cayaponoside A6 162857-59-2P, Cayaponoside B2 162857-60-5P, Cayaponoside B3 162857-61-6P, Cayaponoside D1

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(from *Cayaponia tayuya*)

RN 147742-04-9 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 25-(acetyloxy)-2-(.beta.-D-glucopyranosyloxy)-3,16,20-trihydroxy-4,9,14-trimethyl-,

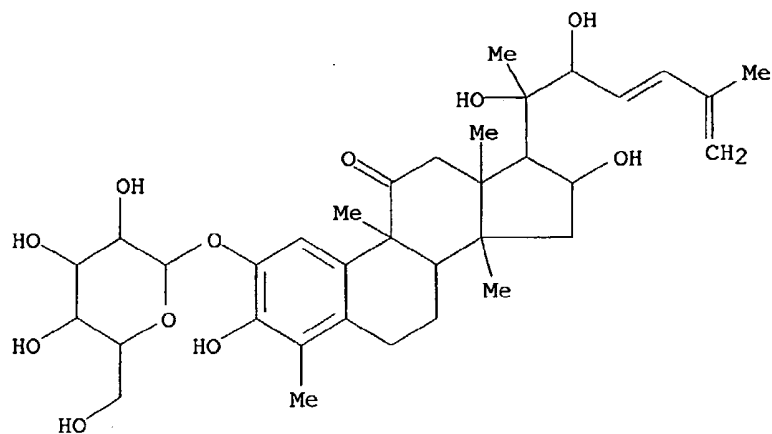
(9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)



RN 147742-05-0 HCAPLUS

CN 19-Norcholesta-1,3,5(10),23,25-pentaen-11-one, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,22-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Currently available stereo shown.



RN 147742-06-1 HCAPLUS

CN 19-Norcholesta-1,3,5(10)-triene-11,22-dione, 2-(.beta.-D-glucopyranosyloxy)-3,16,20,25-tetrahydroxy-4,9,14-trimethyl-, (9.beta.,16.alpha.)- (9CI) (CA INDEX NAME)